

Sliding-Ring Catenanes

Isurika R. Fernando,[†] Marco Frasconi,^{†,§} Yilei Wu,^{†,‡} Wei-Guang Liu,[⊥]
Michael R. Wasielewski,^{†,‡} William A. Goddard III,^{⊥,#} J. Fraser Stoddart*,[†]

[†]Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

[§]Department of Chemical Sciences, University of Padova, Via Marzolo 1, Padova 35131, Italy

[‡]Argonne-Northwestern Solar Energy Research (ANSER) Center, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

[⊥]Materials and Process Simulation Center, California Institute of Technology, Pasadena, California 91125, USA

[#]NanoCentury KAIST Institute and Graduate School of EEWS (WCU), Korea Advanced Institute of Science and Technology (KAIST), 373-1 Guseong Dong, Yuseong Gu, Daejeon 305-701, Republic of Korea

* e-mail: stoddart@northwestern.edu

SUPPORTING INFORMATION

Table of Contents

1. Materials and General Methods.....	S2
2. Solution-State Characterization of [2]Catenanes.....	S3
2.1. UV–Vis Spectroscopy.....	S3
2.2. EPR Spectroscopy.....	S3
2.3. NMR Spectroscopy.....	S4
3. Solid-State Characterization of [2]Catenanes.....	S10
3.1. Crystal Growth.....	S10
3.2. X-Ray Crystallography.....	S11
4. Computational Analysis	S14
5. References.....	S150

1. Materials and General Methods

All reagents were used as received from chemical suppliers (Aldrich and VWR) and reactions were carried out in anhydrous solvents under an inert nitrogen atmosphere, unless otherwise stated. Cyclobis(paraquat-*p*-phenylene) tetrakis(hexafluorophosphate)^{S1} (CBPQT•4PF₆), bisparaphenylene[34]crown-10^{S2} (BPP34C10), 1,5-dinaphtho[38]crown-10^{S3} (DNP38C10), and the catenanes [DNP38C10/CBPQT]•4PF₆^{S4} (**1**•4PF₆) and [BPP34C10/CBPQT]•4PF₆^{S4b,S5} (**2**•4PF₆) were prepared according to previously reported literature procedures with minor modifications. Thin layer chromatography (TLC) was performed on Sigma gel 60 F254 TLC plates (Merck) and chromatograms were viewed under UV light (256 nm and / or 354 nm wavelengths). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). UV–Vis Spectra were obtained on a UV-3600 Shimadzu spectrophotometer. ¹H, ¹³C, ROESY, DOSY and Variable Temperature (VT) Nuclear Magnetic Resonance spectra (NMR) were recorded on a Bruker Avance III spectrometer operating at 600 MHz using deuterated solvents. The temperature (*T*) was calibrated using neat MeOH for *T* < 295K and ethylene glycol for *T* > 295 K for VT–NMR. Chemical shifts (δ) were reported in ppm relative to signals corresponding to the residual non-deuterated solvents (C₆D₅CD₃: δ 2.09 ppm and CD₃CN: δ 1.94 ppm). High resolution mass spectra (HRMS) were recorded on an Agilent 6210 Time of Flight (TOF) LC-MS, employing an electrospray ionization (ESI) source, coupled with an Agilent 1100 HPLC stack using direct infusion (0.6 mL min⁻¹). Electron Paramagnetic Resonance (EPR) measurements were performed at room temperature using a Bruker Elexsys E580 X-band (9.5 GHz) EPR spectrometer, outfitted with variable Q split ring resonator (ER-4118X-MS5-W1). All samples employed in NMR, UV–Vis and EPR experiments were prepared inside an Ar-filled glovebox and the measurements were carried out immediately after sample preparations. Solvents were degassed by purging them with Ar gas during 2 h prior to transferring them to the glovebox. Bis(cyclopentadienyl)cobalt(II), known as cobaltocene (CoCp₂), was purchased from Sigma-Aldrich and assayed in dried and degassed MeCN using a colorimetric method prior to titration experiments. The different oxidation states — 3+, 2+, 1+

and 0 — of the catenanes **1**•4PF₆ and **2**•4PF₆ were obtained by adding 1.0, 2.0, 3.0 and 4.0 equiv of CoCp₂, respectively, in MeCN solutions: they were characterized simultaneously using UV–Vis and EPR spectroscopies. In the cases of UV–Vis and EPR experiments, MeCN was used as the solvent, while NMR spectra were recorded in C₆D₅CD₃ or CD₃CN. Single crystal X-ray diffraction analysis of the [2]catenanes in their 3+ to 0 oxidation states — **1**⁰, **2**⁰, **1**^{•/3+} and **2**^{•/3+} — were performed on a Bruker Kappa Apex II CCD diffractometer using Cu-Kα (λ = 0.15418 nm) radiation at 100 K. Structure solutions and refinements were carried out using the Olex 2 1.2 suite of programs. Data collection and structure refinement details are available in CIF files. CCDC depositions X1, X2, X3 and X4 contain the supplementary crystallographic data for this manuscript and can be obtained free of charge from the www.ccdc.cam.ac.uk/data_request/cif website.

2. Solution-State Characterization of [2]Catenanes

2.1. UV–Vis Spectroscopy

A series of solutions with the catenanes in their 3+, 2+, 1+ and 0 oxidation states were prepared by the chemical reduction of the fully oxidized catenanes using 1.0, 2.0, 3.0 and 4.0 equiv of CoCp₂, respectively. The UV–Vis spectra were recorded in solutions with 1:0, 1:1, 1:2, 1:3 and 1:4 molar ratios of the catenane:CoCp₂ in a final volume of 1.00 mL by using catenane (100 μM) and CoCp₂ (1.7 mM) solutions in MeCN. UV–Vis Spectra of solutions of **1**•4PF₆ and **2**•4PF₆ at different oxidation states (from 4+ to 0) were recorded in the 300–800 nm wavelength window using a 2 mm quartz cuvette.

2.2. EPR Spectroscopy

Samples for EPR investigations were prepared as described for the carrying out of the UV–Vis spectroscopy with the exception that the concentration of the stock solution of catenane was maintained at 250 μM. The EPR spectra of **1**•4PF₆ and **2**•4PF₆ and their reduced states — 3+ to 0 — were recorded at 298 K after the chemical reduction with different equiv of CoCp₂.

2.3. NMR Spectroscopy

For NMR spectroscopic characterization, samples of the catenanes **1**⁰ and **2**⁰ were prepared by extraction from a heterogeneous two-phase system. All the experiments were performed in an Ar glovebox as follows. The chloride salts **1**·4Cl (12.00 mg, 7.3 μmol) and **2**·4Cl (10.00 mg, 8.3 μmol) were dissolved in an aqueous buffer (CO₃²⁻/HCO₃⁻) at pH 9.0 (1.00 mL). The organic phase consisting of C₆D₅CD₃ (1.00 mL) was added to the buffered solution. After adding activated zinc dust as a reducing agent, the bilayer mixture was stirred at room temperature for 30 min. The initial color intensities of the aqueous layers — violet for **1**·4Cl and red for **2**·4Cl, respectively — decreased gradually while the colors of the C₆D₅CD₃ layers changed from colorless to light yellow, followed by a dark yellowish-orange color, indicating that the fully reduced catenanes had been extracted into the C₆D₅CD₃ layers. After washing with H₂O (3 x 1.00 mL), the organic layers were transferred in a Wilmad NMR tube and capped. ¹H, ¹³C, ROESY, DOSY and VT-NMR spectroscopies were performed. See Figure S1 for proton assignments in the ¹H NMR spectra.

1⁰: ¹H NMR (600 MHz, C₆D₅CD₃, 298 K) δ 8.02 (br, 4H, H_{4/8}), 7.20 (br, 4H, H_{3/7}), 7.10 (s, 8H, H_{Xy}), 6.47 (br, 4H, H_{2/6}), 5.28 (br, 8H, H_{α/β}), 3.96 (br, OCH_{2a}), 3.60-3.55 (m, OCH_{2b-d}, N-CH₂).

2⁰: ¹H NMR (600 MHz, C₆D₅CD₃, 298 K) δ 7.22 (br, 8H, H_{Xy}), 6.57 (s, 8H, H_{HQ}), 5.43 (br, 8H, H_α), 5.31 (br, 8H, H_β), 3.85 (t, *J* = 5.4 Hz, 8H, OCH_{2a}), 3.65 (br, 8H, N-CH₂), 3.57 (t, *J* = 5.4 Hz, 8H, OCH_{2b}), 3.53 (s, 16H, OCH_{2c,d}).

In order to evaluate the molecular dynamics of **2**⁰ and compare it with its fully-oxidized counterpart **2**⁴⁺ in solution, VT-NMR spectroscopy (Figure S2) was performed. In the case of both **1**⁰ and **1**⁴⁺, peak broadening, coalescence and reappearing with sharpening of the ¹H NMR resonances were observed (Figures S2 and S3) with changes in temperature. The VT-NMR spectra of **1**⁰ in C₆D₅CD₃ show only a one set of peaks for both rings indicating that the DNP38C10 and CBPQT⁰ rings are undergoing fast rotation on the ¹H NMR time-scale. By contrast, the rings in **1**⁴⁺ undergo slow circumrotations on the ¹H NMR time-scale. See also ref S2.

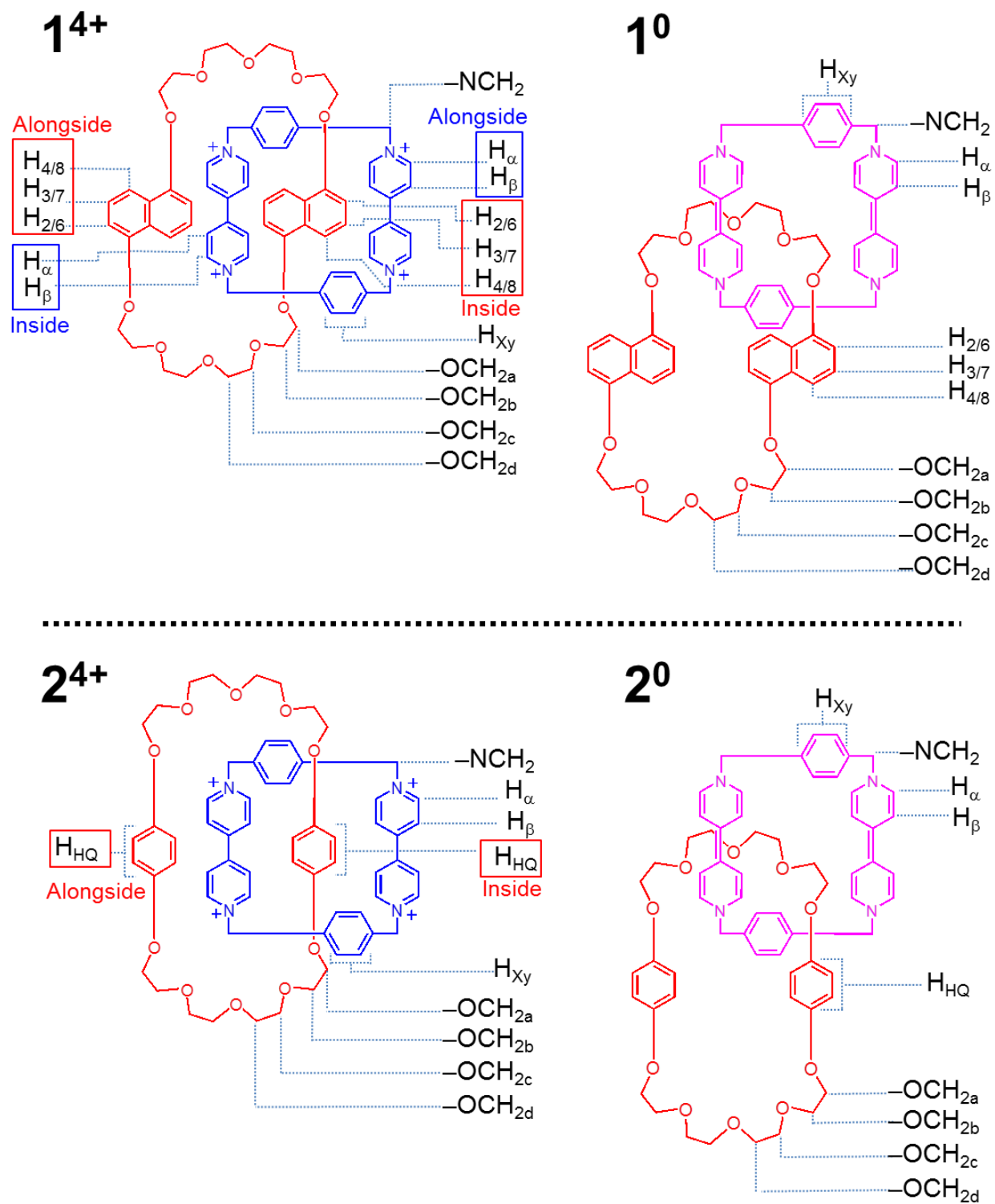


Figure S1. Proton labels on the structural formulas of the [2]catenanes **1⁴⁺**, **1⁰**, **2⁴⁺** and **2⁰**.

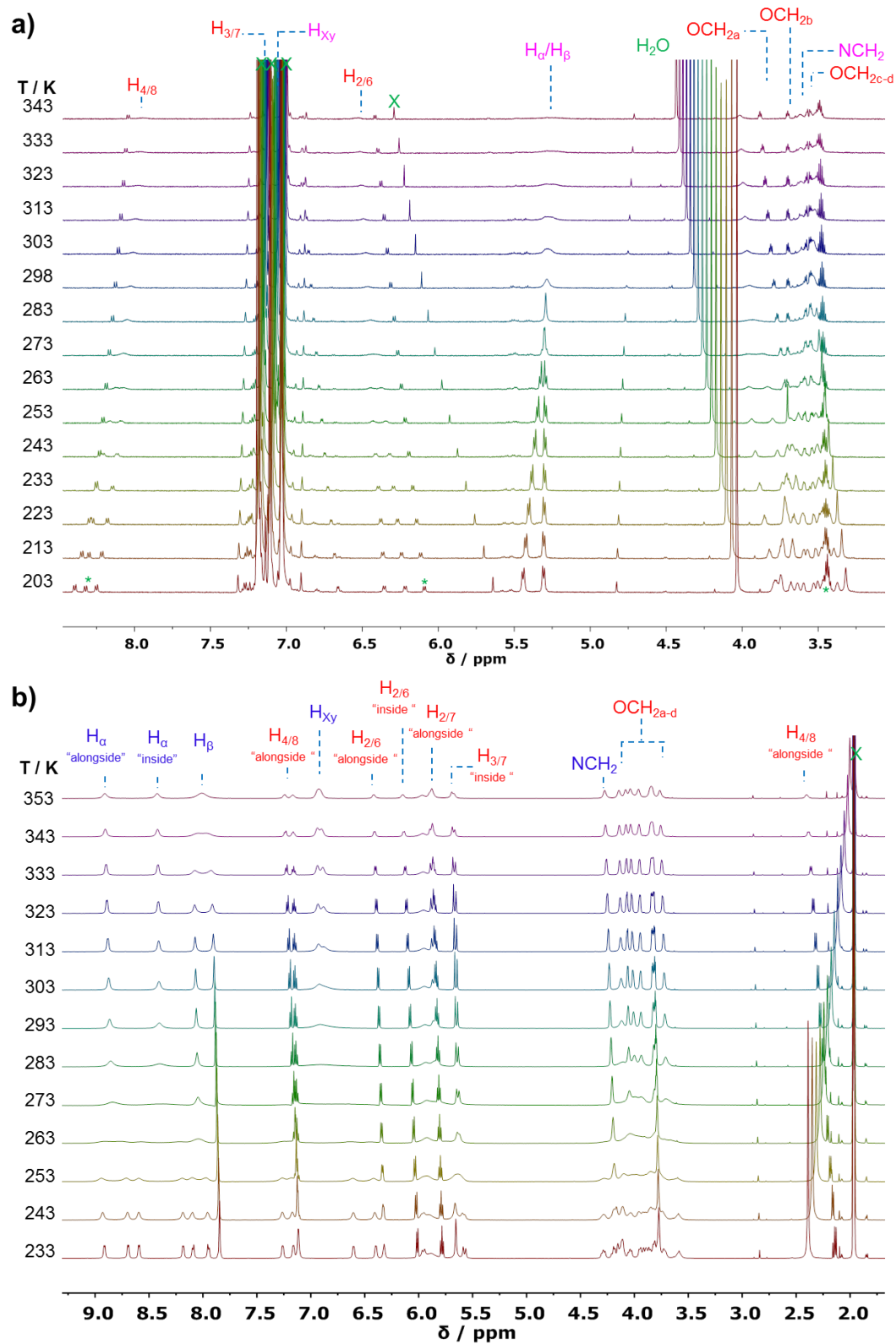


Figure S2. Variable temperature ^1H NMR spectra (600 MHz) of (a) $\mathbf{1}^0$ recorded in $\text{C}_6\text{D}_5\text{CD}_3$ and (b) $\mathbf{1}^{4+}$ recorded in CD_3CN .

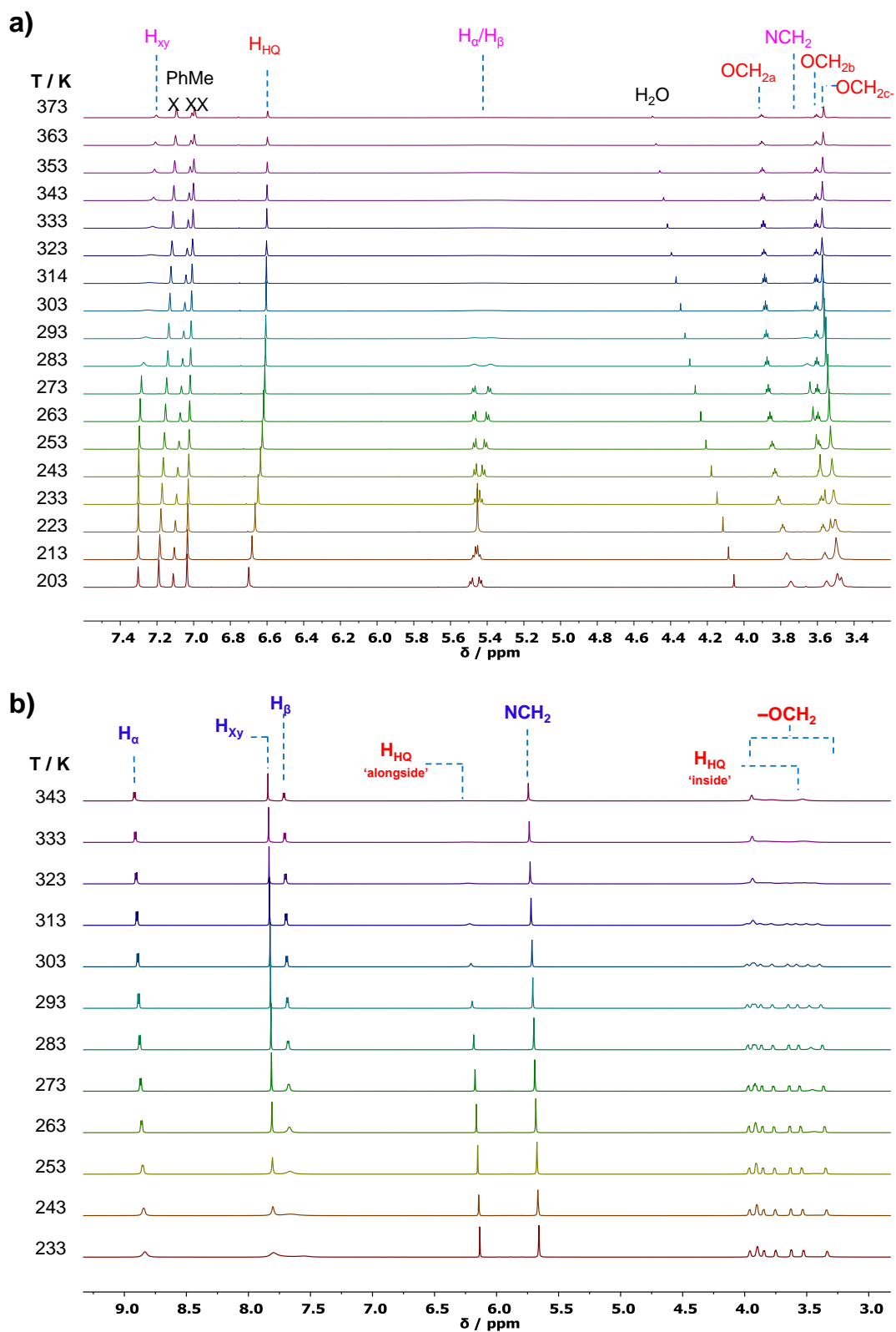


Figure S3. Variable temperature ^1H NMR spectra (600 MHz) of (a) 2^0 recorded in $\text{C}_6\text{D}_5\text{CD}_3$ and (b) 2^{4+} recorded in CD_3CN .

^1H DOSY (Figure S4 and S5) and ^1H - ^1H ROESY (Figure S6 and S7) NMR spectra of $\mathbf{1}^0$ and $\mathbf{2}^0$ were performed at low temperature (248 K) to minimize the molecular-level dynamic phenomena.

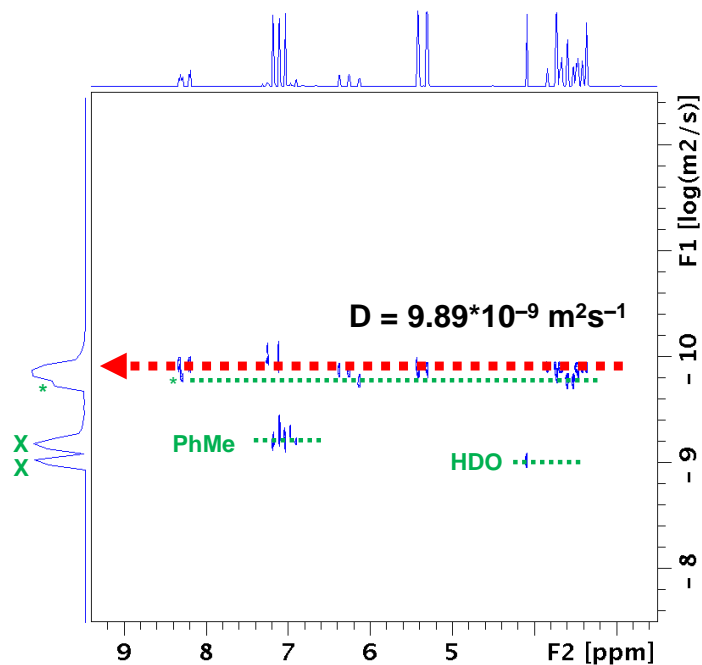


Figure S4. ^1H DOSY NMR spectrum of (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 248 K) of $\mathbf{1}^0$. *The sample contains small amount of DNP38C10 impurities.

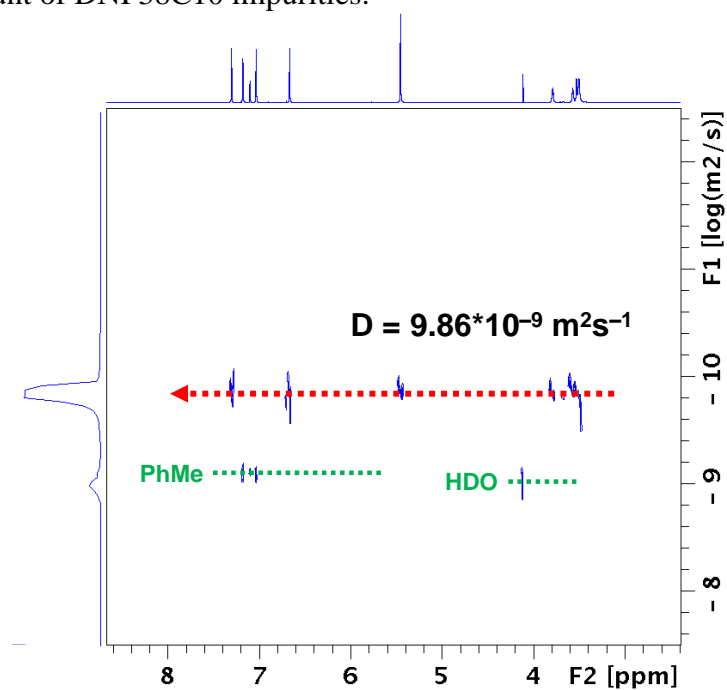


Figure S5. ^1H DOSY NMR spectrum of (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 248 K) of $\mathbf{2}^0$.

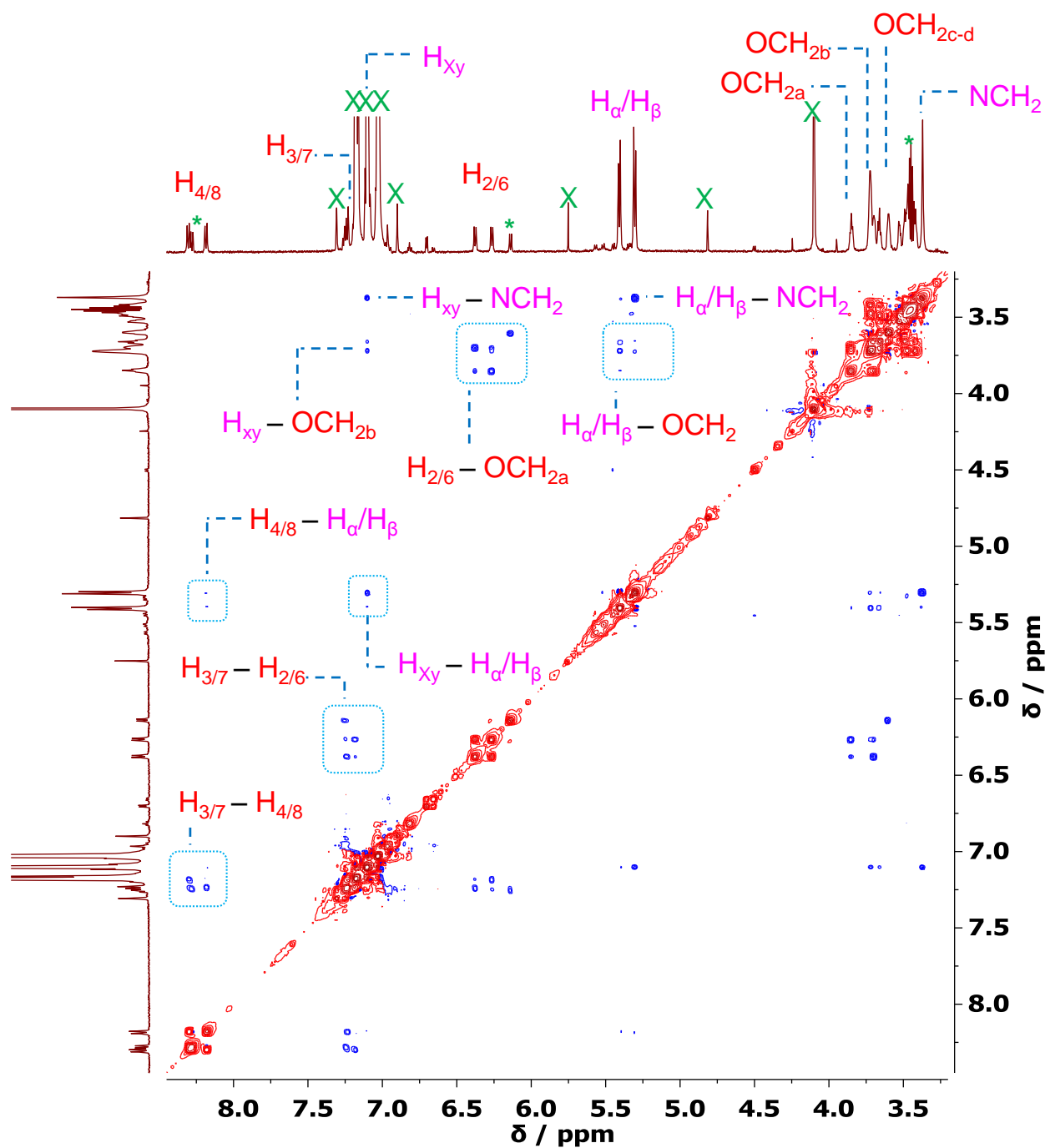


Figure S6. ^1H - ^1H ROESY spectrum of (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 248 K) of **10**.

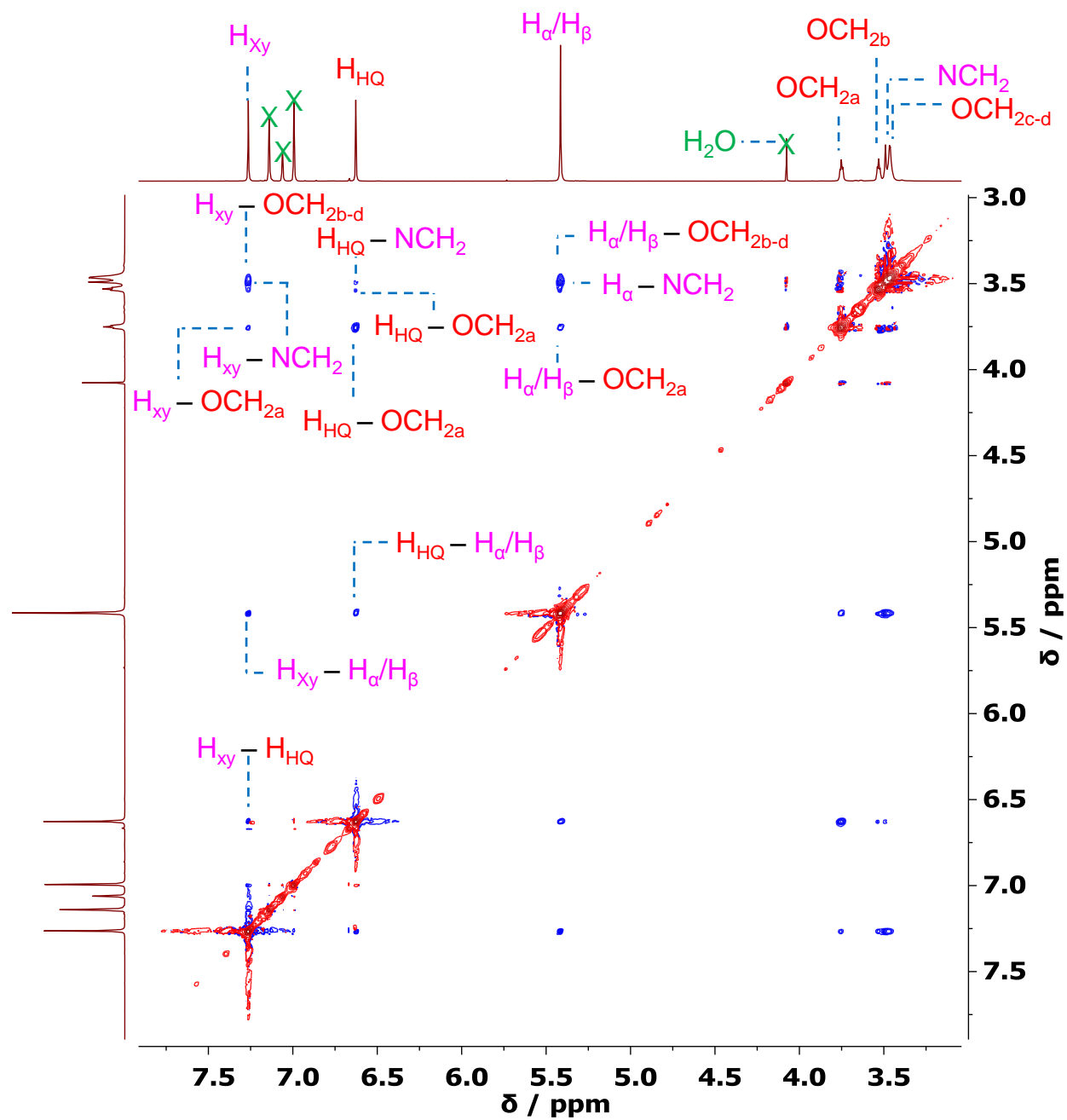


Figure S7. ^1H - ^1H COSY spectrum of (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 248 K) of 2^0 .

3. Solid-State Characterization of [2]Catenanes

3.1. Crystal Growth

Unless otherwise stated, the crystals of [2]catenanes in the different oxidation states were grown in an Ar glovebox at 273 K.

1⁰: **1•4PF₆** (4.75 mg, 2.7 mmol) were dissolved in MeCN (1.00 mL) and 5.0 equiv of saturated CoCp₂ (110 μ L) in MeCN were added. The solution was filtered. After 1 h standing at room temperature, dark orange colored elongated cubes of **1⁰** were obtained in quantitative yield. Vapor diffusion of ⁱPr₂O into a dilute solution of the fully reduced **1⁰** catenane in MeCN yielded the same single crystal of **1⁰** as confirmed by the unit cell parameters.

2⁰: A solution of **2⁰** in PhMe was obtained using a bilayer extraction method, starting with **2•4Cl** (5.00 mg, 3.0 mmol) as explained in *Section 2.3* for the sample preparation prior to NMR spectroscopic investigations. Diffusion of *n*-hexane vapor into a solution of **2⁰** in PhMe yielded bright orange-colored elongated cubic-shaped single crystals of **2⁰** in quantitative yield.

1•3PF₆: **1•4PF₆** (3.30 mg, 1.9 mmol) were dissolved in MeCN (660 μ L) and reduced with activated Zn dust. After 30 min of stirring at room temperature, the solution was filtered and subjected to vapor diffusion with ⁱPr₂O. Within 2 weeks, dark violet-purple colored needles of **1•3PF₆** were obtained in quantitative yield.

2•3PF₆: **2•4PF₆** (3.50 mg, 2.1 mmol) were dissolved in MeCN (660 μ L) and reduced with activated Zn dust. After 30 min of stirring at room temperature, the solution was filtered and subjected to vapor diffusion with ⁱPr₂O. Within 2 weeks, dark violet-purple colored needles of **2•3PF₆** were obtained in quantitative yield.

3.2. X-Ray Crystallography

Table S1: Crystallographic Data for Crystals of 1^0 , 2^0 , $1'^{3+}$ and $2'^{3+}$.

	$1^0 \cdot 2 \text{MeCN}$	$4(2^0 \cdot 1.5 \text{PhMe} \cdot 0.25 \text{H}_2\text{O})$	$1 \cdot 3 \text{PF}_6 \cdot 2 \text{MeCN}$	$2(2 \cdot 3 \text{PF}_6 \cdot 5.5 \text{MeCN})$
Formula	$\text{C}_{76}\text{H}_{82}\text{N}_6\text{O}_{10}$	$\text{C}_{298}\text{H}_{338}\text{N}_{16}\text{O}_{41}$	$\text{C}_{76}\text{H}_{82}\text{F}_{18}\text{N}_6\text{O}_{10}\text{P}_3$	$\text{C}_{150}\text{H}_{177}\text{F}_{36}\text{N}_{19}\text{O}_{20}\text{P}_6$
Formula weight/gmol ⁻¹	1239.47	4799.82	1674.38	3435.92
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	P 12 ₁ /c 1	P -1	C 1 2/c 1	P 1 2 ₁ /n 1
<i>a</i> /Å	13.9493(8)	20.1201(9)	21.9335(5)	19.1189(5)
<i>b</i> /Å	48.567(3)	26.1627(12)	13.4484(3)	19.7795(6)
<i>c</i> /Å	10.9451(5)	26.4880(12)	27.6224(6)	45.0588(12)
α /deg	90.00	87.674(3)	90.00	90.00
β /deg	112.934(3)	69.262(2)	113.1366(7)	93.421(2)
γ /deg	90.00	78.983(3)	90.00	90.00
<i>V</i> /Å ³	6829.0(6)	12793.9(10)	7492.5(3)	17009.2(8)
<i>Z</i>	4	2	4	4
<i>D</i> _{calc} /gcm ⁻³	1.206	1.246	1.484	1.342
$\mu(\text{CuK}\alpha)$ /mm ⁻¹	0.642	0.660	1.685	1.509
Reflns collected/unique	20417 / 9824	83250 / 43042	56084 / 6377	128195 / 28831
Obsd reflns [<i>I</i> > 2σ(<i>I</i>)]	6648	27965	6276	22524
GOF (on <i>F</i> ²)	1.067	1.034	1.047	1.041
<i>R</i> (<i>F</i>), <i>R</i> _w (<i>F</i>) [<i>I</i> > 2σ(<i>I</i>)]	0.1095, 0.2433	0.0849, 0.2244	0.0408, 0.1037	0.0749, 0.2042
CCDC Number	1479750	1479752	1479755	1479751

The extended solid-state superstructure consisting of the cell unit of 2^0 is shown in Figure S8.

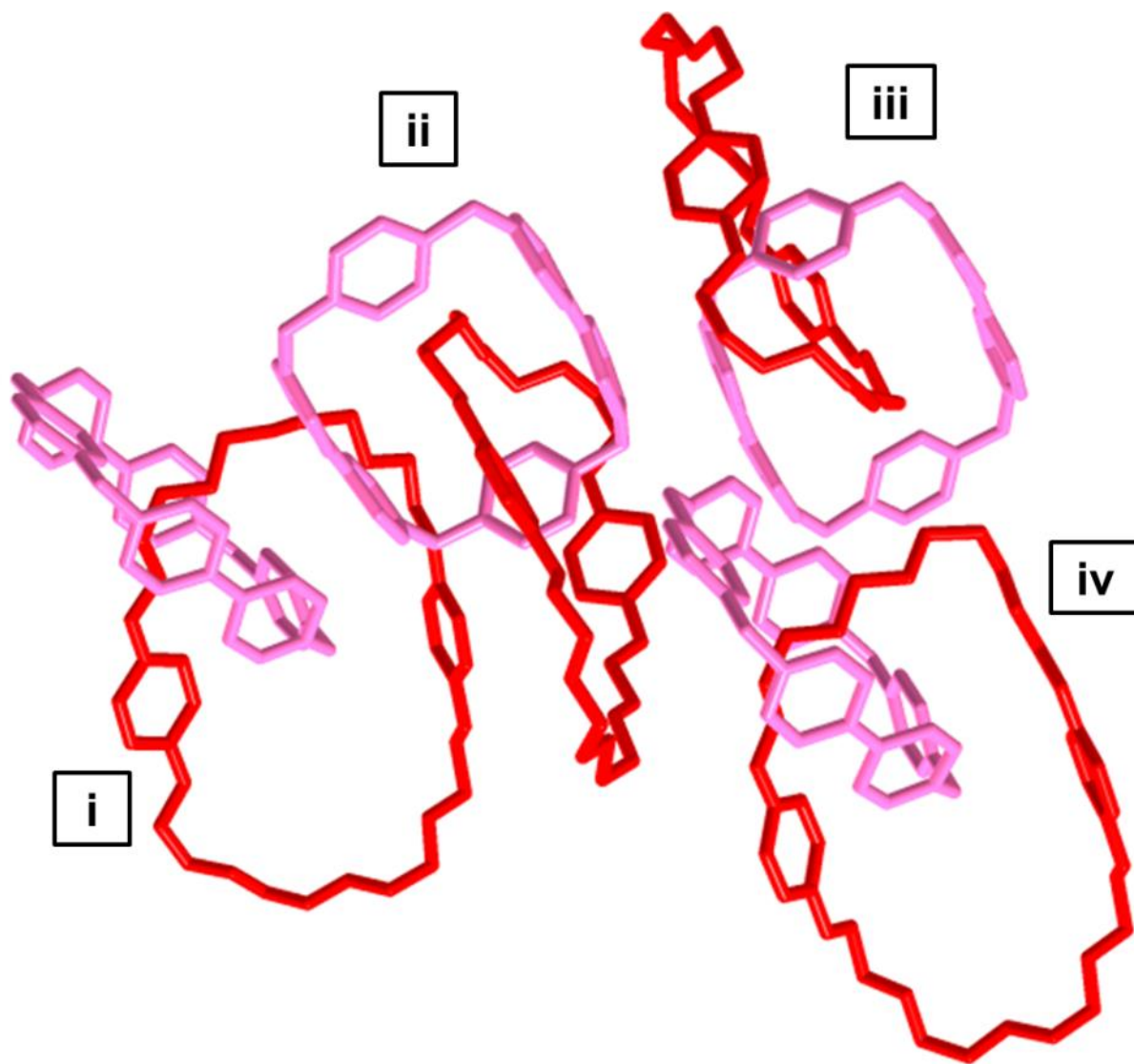


Figure S8. Plan view of the superstructure presents in the unit cell of the 2^0 catenane in a tubular representation displaying the four different co-conformations of the catenane.

Four different co-conformations of the neutral catenane 2^0 are present in the unit cell. In two co-conformations (Figure S9, ii and iii) the BIPY 0 unit of the CBPQT 0 sits around the first CH $_2$ –O–CH $_2$ linker of the glycol chain, while in the other two co-conformations (Figure S9, i and iv) the ring sits on the second CH $_2$ –O–CH $_2$ linker of the glycol chain.

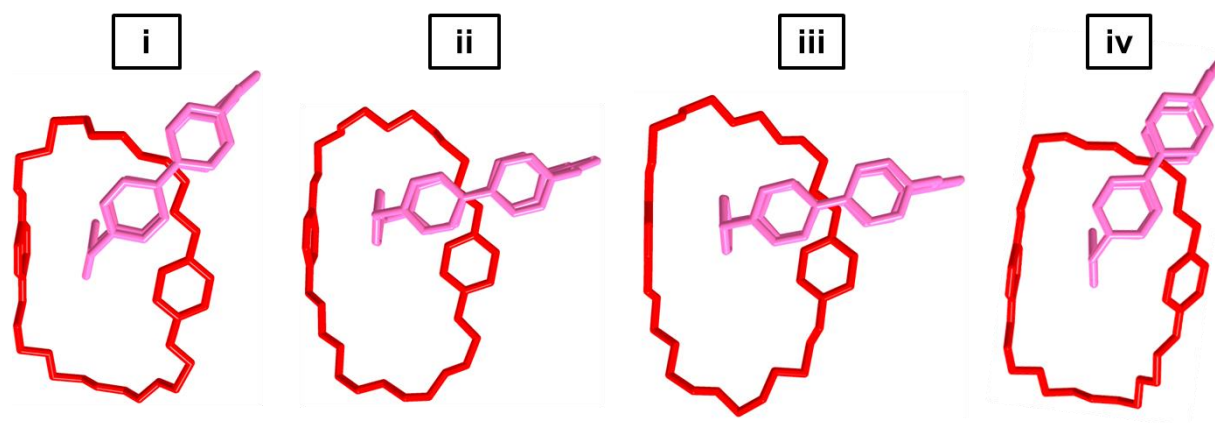


Figure S9. Side-on views of the tubular representation of the four co-conformations present in the unit cell of the 2^0 catenane.

4. Computational Analysis

In order to examine the stability of catenanes resulting from chemical reduction, quantum-mechanical modeling was performed. Density functional theory (DFT) calculations at the level of M06-HF/6-311++G**//M06-HF/6-31G* were employed in order to obtain the predicted geometries of the 4+ to 0 redox states of the catenanes 1^{4+} and 2^{4+} with Poisson-Boltzmann solvation model.

The TD-DFT calculations were carried out on the truncated models of 1^{4+} and 2^{4+} , obtained by removing the glycol chain following re-optimization of the structure at the level of BLYP+LC ($\mu=0.2$)/6-31G(d), which was found to predict accurate excitation energy of the complex between the CBPQT and tetrathiafulvalene (TTF).^{S7} The strongest absorption below 450 nm for both complexes corresponds to the HOMO (located on the electron-rich guests) to LUMO and LUMO+1 (located on the electron-poor CBPQT⁴⁺ ring), as illustrated in Figure S10. The excitation energies for 1^{4+} and 2^{4+} are 557 and 530 nm.

The energy decomposition analysis was carried out with Q-Chem 4.1.0.1^{S8} at M06-HF/6-311G**//M06-HF/6-31G* level.

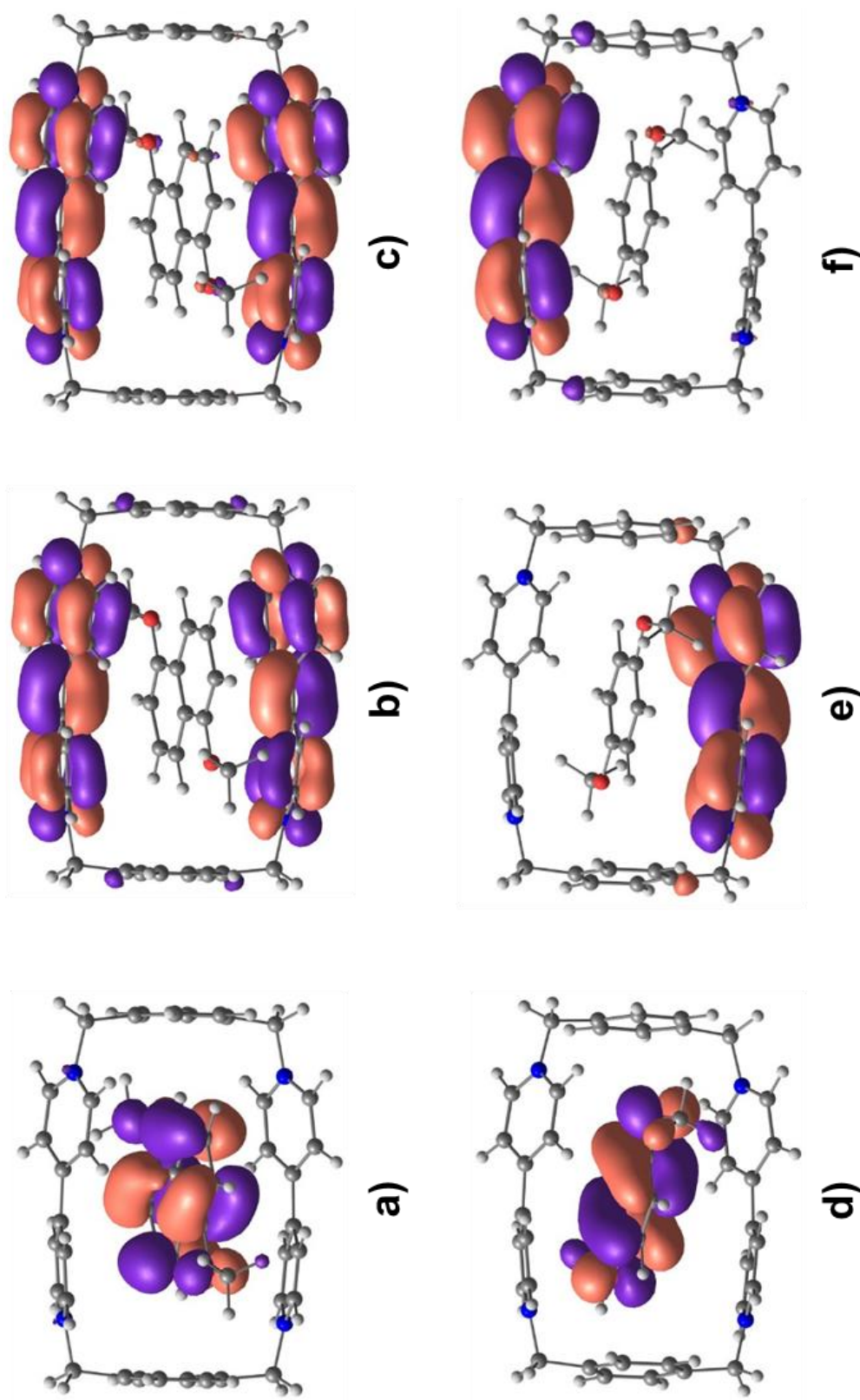


Figure S10. The molecular orbitals involved in the excitations of 1^{4+} and 2^{4+} (truncated models). HOMO (a), LUMO (b) and LUMO+1 (c) of 1^{4+} . HOMO (d), LUMO (e) and LUMO+1 (f) of 2^{4+} .

The energy optimized geometries for the calculated structures $1^{*/3+}$ and $2^{*/3+}$ are shown in Figure S11 and Figure S12, respectively.

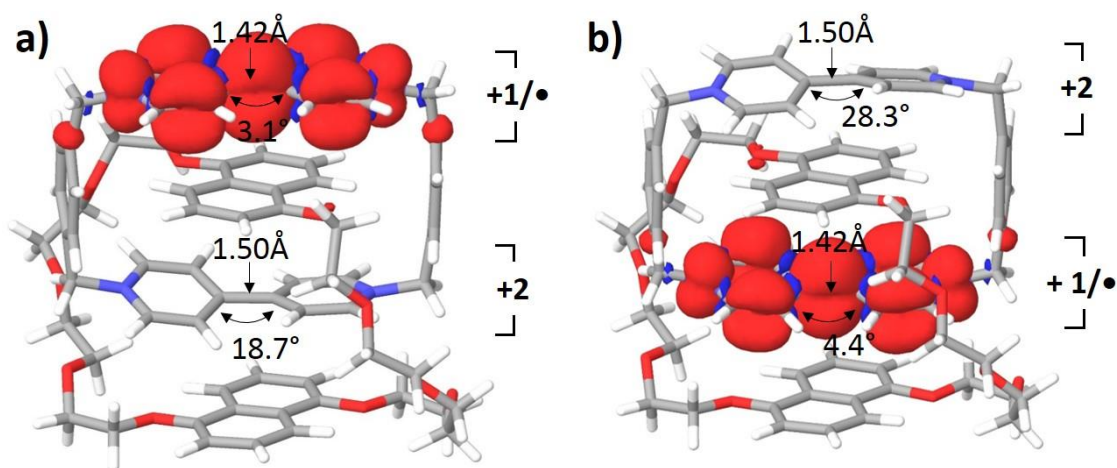


Figure S11. Calculated spin density for two co-conformations of $1^{*/3+}$. (a) The lower-energy co-conformation with the radical cationic BIPY $^{*+}$ alongside and the dicationic BIPY $^{2+}$ inside the DNP38C10 ring. (b) The higher-energy co-conformation (5 kcal mol $^{-1}$) with the radical cationic BIPY $^{*+}$ inside and the dicationic BIPY $^{2+}$ outside the DNP38C10 ring. The bond lengths and the torsional angles around the C4-C4' bond of the BIPY units are shown.

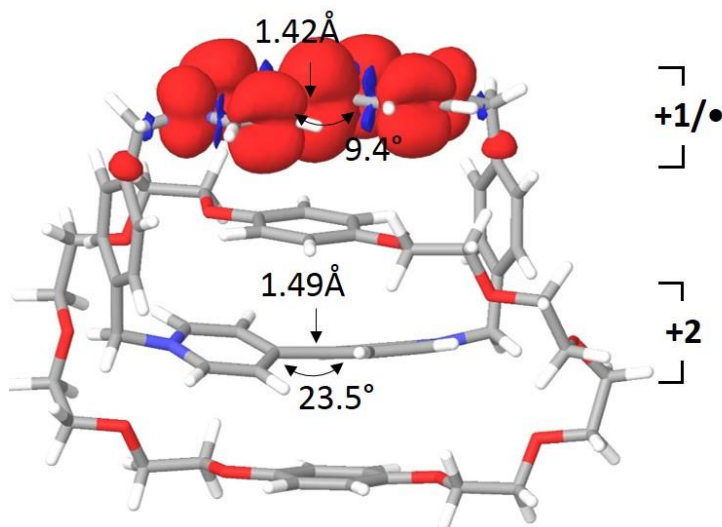


Figure S12. Calculated spin density for the co-conformations of $2^{*/3+}$ with the radical cationic BIPY $^{*+}$ alongside and the dicationic BIPY $^{2+}$ inside the macrocyclic polyether. The reverse co-conformation with the radical cationic BIPY $^{*+}$ inside and the dicationic BIPY $^{2+}$ outside the macrocycle is unstable regardless the initial geometries choose and it converges to the former conformation. The bond lengths and the torsional angles around the C4-C4' bond of the BIPY units are shown.

The calculated structures for two co-conformation of the catenanes $\mathbf{1}^{2(++)}$ (a, b) $\mathbf{2}^{2(++)}$ (Figure S13) show that the diradical dicationic CBPQT $^{2(++)}$ rings encircle the aromatic units of crown ethers.

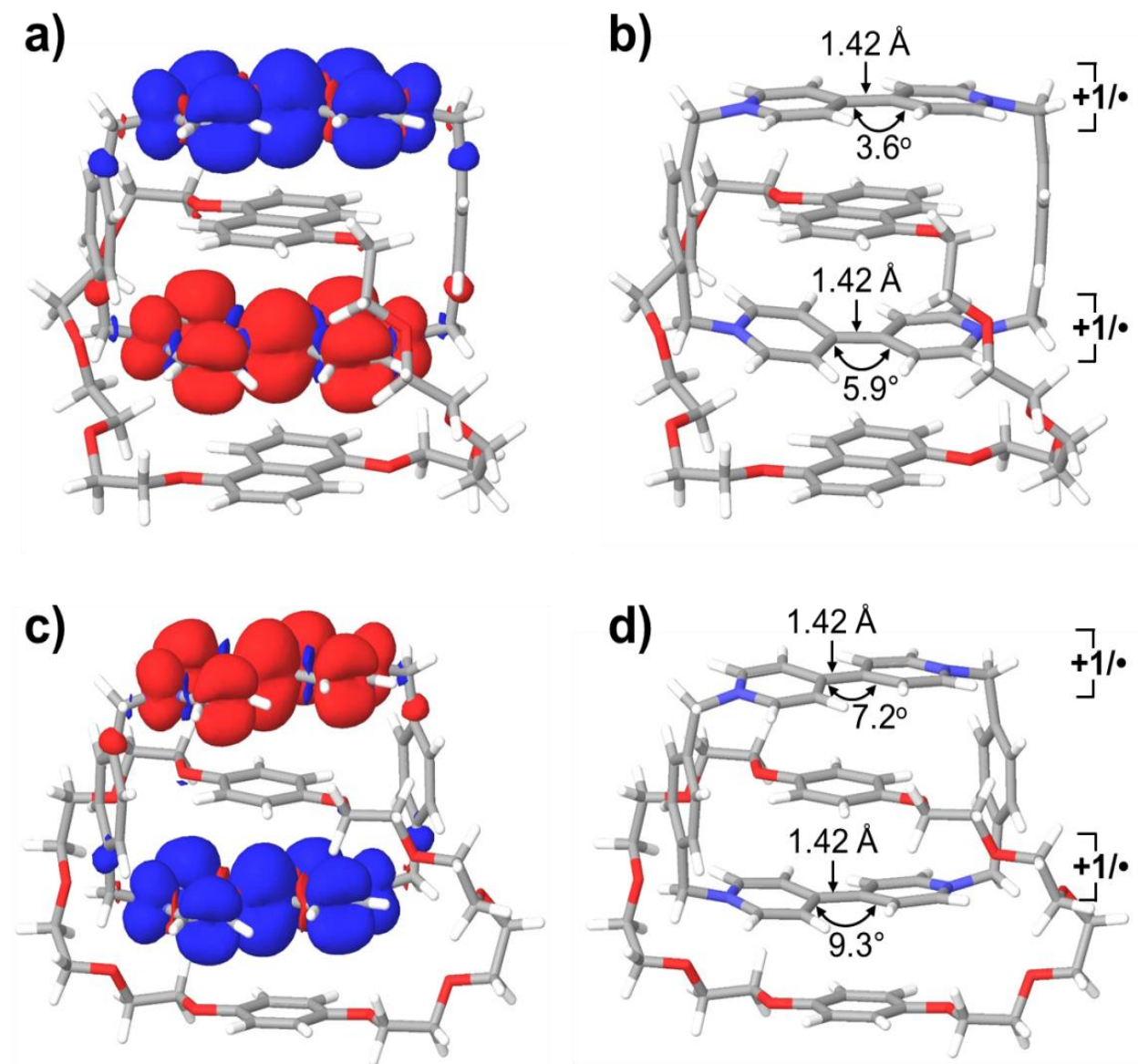


Figure S13. Calculated spin density for two co-conformations of $\mathbf{1}^{2(++)}$ (a, b) $\mathbf{2}^{2(++)}$ (c, d). Spin population of $\mathbf{1}^{2(++)}$ (a) and $\mathbf{2}^{2(++)}$ (c). Calculated geometries of $\mathbf{1}^{2(++)}$ (b) and $\mathbf{2}^{2(++)}$ (d) showing the bond lengths and the torsional angles around the C4–C4' bond of the BIPY units.

The energy optimized geometries for the calculated structures of 1^{*+} and 2^{*+} are shown in figure S14 and S15, with bond distances and torsional angles around the C4–C4' bond of the BIPY units.

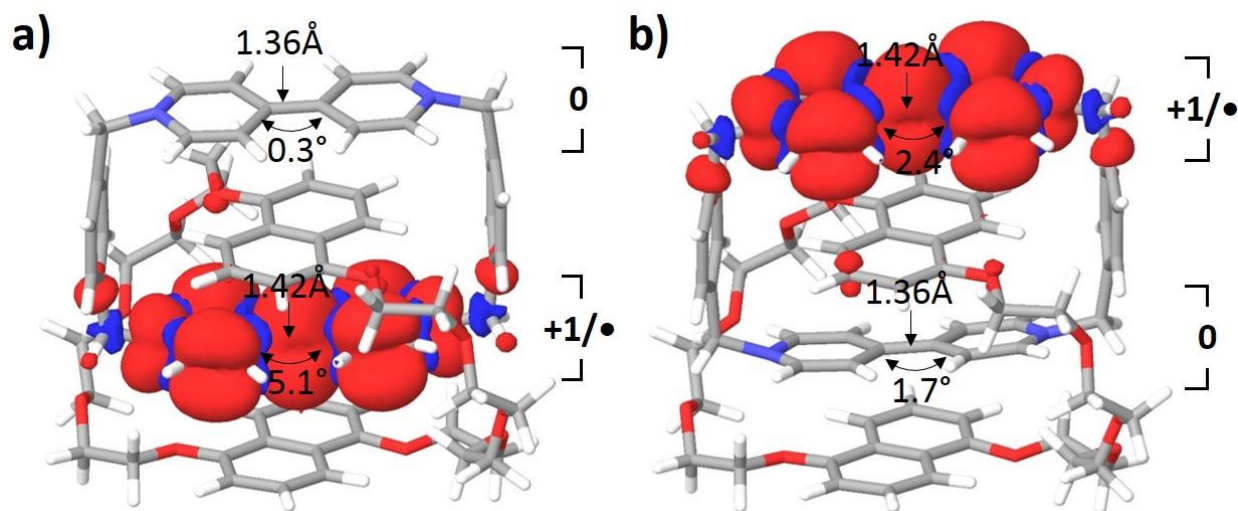


Figure S14. Calculated spin density for two co-conformations of 1^{*+} . (a) The lower-energy co-conformation with the radical cationic BIPY^{•+} located inside the DNP38C10 ring. (b) The higher-energy co-conformation (9.3 kcal mol⁻¹) with the radical cationic BIPY^{•+} located outside the DNP38C10 ring. The bond lengths and the torsional angles around the C4–C4' bond of the BIPY units are shown.

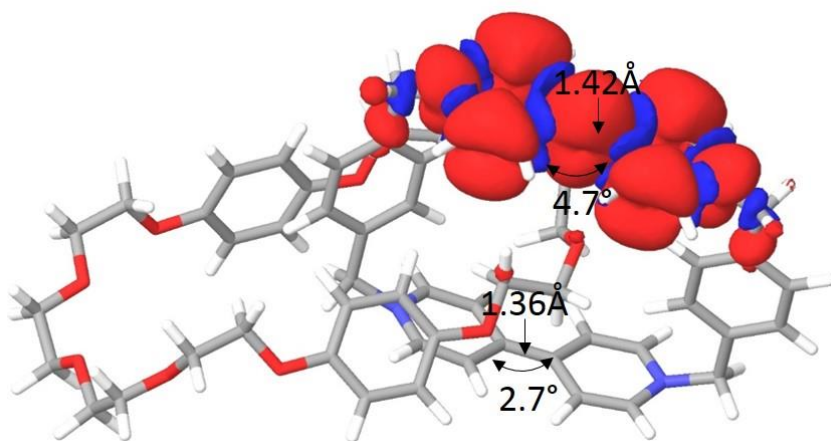


Figure S15. Calculated spin density of 2^{*+} with the radical cationic BIPY^{•+} alongside and the dicationic BIPY²⁺ inside the macrocyclic polyether.

In order to investigate the stability of the neutral catenanes 1^0 and 2^0 in different conformations, the potential energy surface for the sliding of the CBPQT ring through the crown ether was compared (Figure S16) to the energy for the movement of the CBPQT^{4+} ring in the fully oxidized catenane.

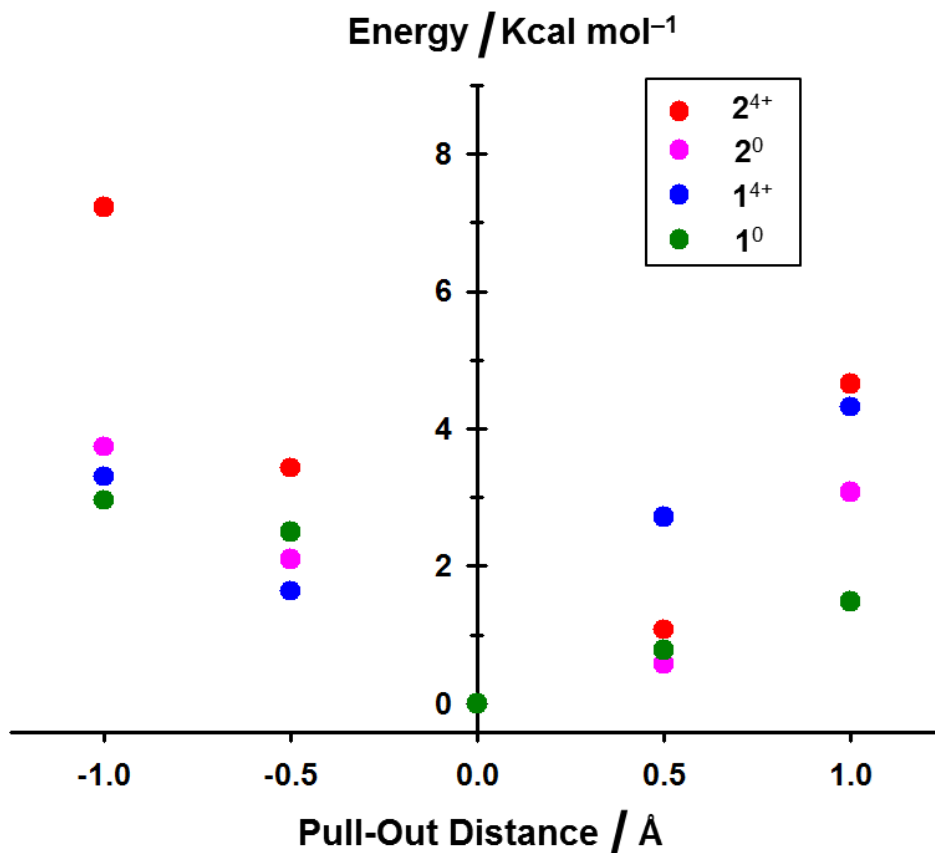


Figure S16. Potential energy surface calculated for the sliding of the CBPQT ring through the crown ether for the neutral and tetracationic catenanes 1^{4+} and 2^{4+} . The potential energy surfaces of the neutral and tetracationic catenanes at different conformations were calculated by pushing away the CBPQT ring from the equilibrium position by 0.5 and 1.0 Å in the direction perpendicular to the plane defined by the carbons in four ethylene units and then optimized with all other coordinates relaxed.

The coordinates of optimized complexes were reported in XYZ format. The energies were reported in the following format: (1) M06-HF/6-31G* (in solution), (2) M06-HF/6-31G* (in gas phase), (3) M06-HF/6-311++G** (in gas phase), and (4) the total energy, which is (1)-(2)+(3).

1⁴⁺ CBPQT circling DNP

-3759.127058 -3758.479648 -3759.497667 -3760.145077

O1	8.4307055988000	13.9187421606000	5.0742991740000
C2	9.8227822705000	14.1547583580000	4.8957210800000
C3	7.9569284090000	13.9810048832000	6.3459677018000
C4	10.2049349068000	13.9637093546000	3.4387820486000
C5	6.5342234168000	13.8147398869000	6.4831825336000
C6	8.7374838604000	14.2060259501000	7.4545073909000
O7	9.5930945679000	14.9470852556000	2.6163921975000
C8	5.7085942937000	13.5712254046000	5.3501355055000
C9	5.9612611933000	13.9261755626000	7.7667855226000
C10	8.1336613049000	14.2915023073000	8.7391244330000
C11	10.3581194201000	15.2818831677000	1.4611097174000
C12	4.3530829659000	13.4877192402000	5.5123591480000
C13	4.5364683983000	13.7854161834000	7.9022481470000
C14	6.7814115693000	14.1699303557000	8.9042912532000
C15	9.4095001341000	15.5667448321000	0.3006979645000
C16	3.7474058862000	13.6026617501000	6.7923845596000
O17	4.0836752128000	13.8384965996000	9.1788484926000
O18	8.4236873921000	16.5355794600000	0.6157421176000
C19	2.6869297100000	13.7091091812000	9.4137344930000
C20	8.8933628292000	17.8713258854000	0.7298809311000
C21	1.9435342632000	15.0212603529000	9.1824924866000
C22	7.7525421052000	18.8137796213000	0.3838749862000
O23	2.2608762779000	15.8825314759000	10.2568688169000
O24	6.7108257664000	18.6539615605000	1.3322798967000
C25	1.6123470254000	17.1368833449000	10.1872041633000

C26	5.7250235611000	19.6618348103000	1.2043000588000
C27	1.7192571399000	17.7928448888000	11.5528282804000
C28	4.7129340068000	19.5241169299000	2.3303873990000
O29	3.0926062802000	17.8890214147000	11.8948046997000
O30	5.4420277270000	19.6082814597000	3.5448044072000
C31	3.3325387187000	18.5910780202000	13.1068751145000
C32	4.7933374396000	19.8630967723000	4.7051991873000
C33	3.6059912899000	20.0638568403000	12.8271142233000
C34	5.6655975602000	20.1573684488000	5.8068639920000
C35	3.4330035685000	19.8327108597000	4.8734281900000
O36	4.7507247703000	20.1154739277000	11.9964400108000
C37	7.0785145415000	20.2106165286000	5.6273860785000
C38	5.0962787830000	20.3938836757000	7.0716858039000
C39	2.8823415252000	20.0843962289000	6.1624369364000
C40	5.1485225069000	21.4241594618000	11.6368239846000
C41	7.8810154741000	20.5093989916000	6.6930092348000
C42	5.9764300844000	20.6685017216000	8.1734919085000
C43	3.6809720324000	20.3544151764000	7.2402091748000
C44	6.1151220227000	21.2997362569000	10.4725686192000
C45	7.3344608387000	20.7416826279000	7.9857634764000
O46	5.3550470208000	20.8344098398000	9.3653895751000
H47	10.3995169526000	13.4414533860000	5.4886023342000
H48	10.0690113867000	15.1716293908000	5.2104942982000
H49	11.2930025348000	14.0540474774000	3.3897624255000
H50	9.9191766502000	12.9645174058000	3.1001229115000
H51	9.8076047933000	14.3342516954000	7.3736214243000
H52	6.1644844876000	13.4756424258000	4.3757176400000

H53	8.7724938642000	14.4703160152000	9.5953162316000
H54	10.9915153283000	16.1431442767000	1.6851416808000
H55	10.9971607028000	14.4465928237000	1.1662382702000
H56	3.7127761894000	13.3318024518000	4.6531495887000
H57	8.8681483369000	14.6559915365000	0.0476061576000
H58	9.9919419933000	15.8852751611000	-0.5692199676000
H59	2.5850315954000	13.4429048711000	10.4629095744000
H60	2.2703775609000	12.9065304785000	8.8039661853000
H61	9.7145628113000	18.0450655025000	0.0287884233000
H62	9.2425322931000	18.0710497485000	1.7462736292000
H63	2.2396600123000	15.4704739637000	8.2289597762000
H64	0.8679443843000	14.8215789937000	9.1561366185000
H65	8.1313962543000	19.8401514677000	0.4091216551000
H66	7.3871482175000	18.5939944510000	-0.6237067124000
H67	2.0802186672000	17.7704104548000	9.4248705748000
H68	0.5542220624000	17.0164672584000	9.9370432174000
H69	6.1907279014000	20.6490258826000	1.2718972775000
H70	5.2043614436000	19.5798353912000	0.2453326913000
H71	1.2542042078000	18.7809627281000	11.5124675264000
H72	1.1984248921000	17.1804626704000	12.2925611857000
H73	3.9917417594000	20.3410042262000	2.2577250772000
H74	4.1839424590000	18.5708918011000	2.2718220169000
H75	2.4848423677000	18.4856056917000	13.7877307055000
H76	4.2109137111000	18.1442082456000	13.5739768679000
H77	3.7835883258000	20.5900554359000	13.7702194355000
H78	2.7542377099000	20.5262610377000	12.3197026789000
H79	2.7729035398000	19.6077238357000	4.0462246366000

H80	7.4861412387000	20.0278653655000	4.6425574080000
H81	1.8059582689000	20.0597199870000	6.2776734899000
H82	4.2846446730000	22.0156451804000	11.3221226877000
H83	5.6410661134000	21.9248988576000	12.4749447029000
H84	8.9542178982000	20.5752002578000	6.5666603382000
H85	6.9016179307000	20.5828398830000	10.7230299943000
H86	6.5639630993000	22.2676581529000	10.2407646865000
H87	6.3178113701000	14.2553349426000	9.8792776635000
H88	2.6709190658000	13.5306078253000	6.8644373081000
H89	3.2621767520000	20.5443462864000	8.2187164831000
H90	7.9994860976000	20.9759227428000	8.8057977654000
C91	5.7181300777000	10.2741602342000	6.9988872154000
C92	6.8139140792000	9.9114799869000	6.2076810393000
C93	4.4746415003000	10.4005826258000	6.3759078113000
C94	5.8827883699000	10.5701587522000	8.4589315358000
C95	6.6559562218000	9.7672361590000	4.8420863542000
C96	4.3770532439000	10.2439124349000	5.0043437350000
C97	4.8041978378000	10.5101170490000	9.3474673662000
C98	7.1243320764000	10.9694811364000	8.9602131811000
N99	5.4586906396000	9.9600570370000	4.2638343500000
C100	4.9795722877000	10.8978710057000	10.6639485681000
C101	7.2425134847000	11.3295352383000	10.2891518460000
N102	6.1787792601000	11.3091238157000	11.1070574282000
C103	5.4153982810000	11.4321506389000	2.3134205341000
C104	6.6511826042000	12.0818292459000	2.2326471179000
C105	4.2463823262000	12.1506593255000	2.0661331841000
C106	6.3983723765000	13.3752692994000	12.4036759948000

C107	6.7120780196000	13.4511927985000	1.9889766052000
C108	4.3060440090000	13.5233294508000	1.8126596229000
C109	7.6340880345000	14.0233638925000	12.3960648833000
C110	5.2293134008000	14.1215106304000	12.2318715603000
C111	5.5332597443000	14.1851844407000	1.8114956972000
C112	7.7019559041000	15.3945144801000	12.1445391125000
C113	5.2921398073000	15.4897789980000	11.9770380403000
C114	5.5951777568000	15.7044593886000	1.7114763187000
C115	6.5379544687000	16.1233344184000	11.8987443592000
N116	5.7555483206000	16.2504030536000	3.0941129717000
C117	4.6780518699000	16.3854192285000	3.8815835202000
C118	6.9865626856000	16.4974467811000	3.5643362163000
N119	6.5204208979000	17.6009441788000	9.9568853993000
C120	4.8071678517000	16.7431257159000	5.2079639173000
C121	7.1711668396000	16.8675950604000	4.8875050073000
C122	7.6102764280000	17.4914862437000	9.1882357276000
C123	5.2879991715000	17.6091787922000	9.4154344110000
C124	6.0771993349000	16.9723270494000	5.7517550330000
C125	7.5041411521000	17.3337738162000	7.8141057769000
C126	5.1302388931000	17.4367214950000	8.0555275480000
C127	6.2445436369000	17.2607981396000	7.2194021236000
H128	7.7938955944000	9.7277252522000	6.6254251029000
H129	3.5772681987000	10.6606584391000	6.9181689995000
H130	7.4763912667000	9.4938423608000	4.1937011079000
H131	3.4397127352000	10.3601064763000	4.4777596894000
H132	3.8262528170000	10.1603175603000	9.0476589663000
H133	8.0024277639000	11.0557008655000	8.3357737746000

H134	4.1726687479000	10.8760815631000	11.3827389809000
H135	8.1805286200000	11.6601973891000	10.7129009273000
H136	7.5694651977000	11.5252851655000	2.3840553298000
H137	3.2837952853000	11.6518419908000	2.0813051622000
H138	7.6734949653000	13.9558849273000	1.9954768504000
H139	3.3887636154000	14.0730705521000	1.6347569006000
H140	8.5468084061000	13.4660669422000	12.5749510882000
H141	4.2632321035000	13.6327694814000	12.2778669258000
H142	8.6677847986000	15.8867002968000	12.1253745360000
H143	4.3743093575000	16.0471392080000	11.8104452949000
H144	6.4535067273000	16.0522840588000	1.1405098314000
H145	4.6774201493000	16.1181903067000	1.3001725399000
H146	3.7161028807000	16.1692603315000	3.4364266896000
H147	7.8073486862000	16.3493125830000	2.8725994001000
H148	3.8994259265000	16.8013877667000	5.7878259765000
H149	8.1846778916000	17.0549805482000	5.2112000455000
H150	8.5684778113000	17.5103785126000	9.6897286970000
H151	4.4626942357000	17.7559637613000	10.1057096771000
H152	8.4242701953000	17.2371785500000	7.2572345514000
H153	4.1234863309000	17.4610769804000	7.6688149154000
C154	5.3459305855000	9.9798678885000	2.7686975140000
H155	6.1667114836000	9.3840048329000	2.3774672578000
H156	4.3985291090000	9.5137452505000	2.5094840077000
C157	6.3260553107000	11.8570032202000	12.4962077523000
H158	5.4633406194000	11.5201043305000	13.0650353553000
H159	7.2327316109000	11.4277357554000	12.9161184957000
C160	6.6387657249000	17.5752579580000	11.4475353186000

H161	5.8397146493000	18.2079320290000	11.8288517850000
H162	7.6023078275000	18.0073798335000	11.7071060065000

1³⁺ CBPQT circling DNP (radical sandwiched by two DNP units)

-3759.259517 -3758.857425 -3759.882275 -3760.284367

N1	1.8833148865	9.2221504781	22.4295687531
C2	3.1922568041	9.0456970558	22.1960152292
C3	1.0384095839	9.5250135954	21.4287933660
C4	1.3379370081	8.9478721702	23.7994505869
C5	3.7032048937	9.1207385010	20.9112162230
C6	1.4908747950	9.6193268006	20.1273755495
C7	1.0746685682	7.4524272049	23.9038611853
C8	2.8407078742	9.3803198093	19.8443807954
C9	-0.1198113643	6.9114521614	23.4221231222
C10	2.0643989301	6.5976740441	24.3922625795
C11	3.3320824468	9.3524995469	18.4320279963
C12	-0.2886653005	5.5288640067	23.3476714467
C13	1.8953710210	5.2150243496	24.3186735040
C14	2.4599590339	9.0240119625	17.3929657342
C15	4.6735455159	9.6003534397	18.1201477403
C16	0.7390663580	4.6720841139	23.7544575163
C17	2.9516431064	8.9091568107	16.1057543654
C18	5.1083666578	9.4575694062	16.8163480657
C19	0.6361295426	3.1736109682	23.4911520081
N20	4.2522824946	9.1047351408	15.8420118581
N21	1.2062364436	2.8684454073	22.1632845156
C22	4.7612033258	8.7977004790	14.4654065096

C23	2.5283330486	2.5768761335	22.0159199166
C24	0.4303571080	3.0028397342	21.0519584605
C25	4.8340801498	7.2844464193	14.3145800788
C26	3.1027329512	2.4196593962	20.7898869546
C27	0.9442958679	2.8351646349	19.8005796235
C28	5.8538236854	6.5729552015	14.9523373837
C29	3.8460484933	6.5865684022	13.6198023256
C30	2.3345051976	2.5670070870	19.5891475527
C31	5.8473446743	5.1813155996	14.9619819809
C32	3.8504084939	5.1894233509	13.6116983252
C33	2.9156199372	2.5063378782	18.2907240548
C34	4.8291466111	4.4786816420	14.3084883887
C35	2.1421422230	2.6180447545	17.0898634009
C36	4.3257133683	2.3659238233	18.0829730245
C37	4.7353394023	2.9608455953	14.4456253134
C38	2.7477458210	2.6967137243	15.8735604780
C39	4.8775068420	2.4289785013	16.8389599862
N40	4.1037619099	2.6262529553	15.7350149130
O41	-0.4147994241	5.7958676816	19.6436831344
C42	0.5774693454	5.8531572489	18.7193176769
C43	1.9063015492	5.9270206876	19.2615478692
C44	0.3777812460	5.8276954361	17.3602860832
C45	2.9958411534	5.9482834090	18.3691051512
C46	2.1280501713	5.9362591235	20.6687037444
O47	-2.5355129100	4.5358668413	21.2497618833
C48	2.7773394378	5.9055980675	16.9646152457
C49	4.3262147832	6.0127858923	18.9076222705

C50	3.4095688509	5.9657156064	21.1419288189
O51	5.3154905228	6.0785132397	17.9795404521
C52	4.5262800489	6.0187146887	20.2655917483
C53	-3.4779230218	2.5950298419	22.2443241218
O54	-2.2339532173	1.9410992361	22.4634966878
C55	-2.2634293656	0.5419276128	22.2102862228
O56	7.6413746634	4.0341025617	17.8665800696
C57	-0.8456864524	-0.0061861428	22.1606955380
O58	-0.2369140647	0.0955362880	23.4405686275
C59	8.9796589530	2.1932004452	17.0990420060
C60	0.6792950486	-0.9378954893	23.7574315715
O61	7.9426245080	1.3993558317	16.5539068945
C62	2.0464668855	-0.7728505877	23.0989793851
C63	8.4161197458	0.5157407718	15.5531664298
O64	1.8567729260	-0.8420858664	21.6950946210
C65	7.3611687131	-0.5303379392	15.2469424126
C66	2.9325924452	-0.8101676934	20.8663955707
O67	6.3120774270	0.0498279259	14.4880019966
C68	2.5945703219	-0.7885444658	19.4712349519
C69	4.2413548577	-0.8038851392	21.2728723493
C70	5.3257724416	-0.8919977295	14.0988441676
C71	3.6350990780	-0.7789119121	18.5231846343
C72	4.0357262855	-0.7129929158	14.8837319736
C73	3.2832290064	-0.7816694545	17.1310022333
O74	4.3308833015	-0.8345898760	16.2661496105
H75	3.8171624287	8.8266036082	23.0511367399
H76	0.0040968198	9.6945422235	21.6933309680

H77	2.0823372846	9.2867201854	24.5156092127
H78	0.4312000221	9.5378315928	23.9070359721
H79	4.7585284099	8.9360766015	20.7745369247
H80	0.7802231875	9.8885832791	19.3580746844
H81	-0.9159925814	7.5671634802	23.0876071840
H82	2.9759224182	7.0034553347	24.8174334940
H83	-1.2019425535	5.1161776864	22.9305618485
H84	2.6804701620	4.5622622975	24.6838105436
H85	1.4166001148	8.7944970587	17.5594206216
H86	5.3915369846	9.9098752754	18.8668821196
H87	2.3212180617	8.6340517784	15.2722423104
H88	6.1362850826	9.6308401838	16.5293023073
H89	1.1903976214	2.6017298537	24.2326618428
H90	-0.3979398670	2.8337997806	23.4784614915
H91	4.0687945892	9.2470885397	13.7575502528
H92	5.7363921273	9.2695240814	14.3735232406
H93	3.1007797755	2.4907066243	22.9299700600
H94	-0.6080448307	3.2548361326	21.2288586292
H95	4.1549733499	2.1826762892	20.7646620603
H96	0.2672120273	2.9567556956	18.9675142825
H97	6.6483327407	7.1088327921	15.4591180043
H98	3.0681266716	7.1240966062	13.0890529304
H99	6.6150902800	4.6455438517	15.5108607240
H100	3.0742764242	4.6580485501	13.0724482810
H101	1.0646160606	2.6664714713	17.1099679172
H102	4.9987518073	2.1940682246	18.9085828403
H103	4.1276964460	2.5396608739	13.6453772217

H104	5.7140706317	2.4842401152	14.4324574967
H105	2.1840128837	2.8194095778	14.9581181891
H106	5.9416293254	2.3139901715	16.6698611928
H107	-0.6172721113	5.7666167503	16.9414006826
H108	1.2811047535	5.8948209228	21.3388900286
H109	3.6319368887	5.8929585144	16.3005988907
H110	3.5928075509	5.9408143613	22.2082822869
H111	5.5190585633	6.0488776979	20.6932985996
H112	-4.2852653086	1.8656498813	22.1504859636
H113	-3.6820496986	3.2407652208	23.0989293236
H114	-2.8332554642	0.0325238041	22.9945463918
H115	-2.7341156313	0.3413784371	21.2415686156
H116	-0.2624267066	0.5442981508	21.4209427589
H117	-0.9087006517	-1.0565771725	21.8582595115
H118	9.8007451739	1.5507559097	17.4322279411
H119	9.3624900554	2.8985879554	16.3557262945
H120	0.8224119587	-0.9157493402	24.8374751191
H121	0.2632051548	-1.9099278939	23.4774117839
H122	2.4926742399	0.1862329237	23.3666563631
H123	2.6959578012	-1.5845804903	23.4369864485
H124	8.6727826757	1.0641270245	14.6421494433
H125	9.3095038439	-0.0033820606	15.9146041704
H126	6.9742481868	-0.9422694681	16.1797850846
H127	7.8329418007	-1.3317398292	14.6704760224
H128	4.5008316780	-0.8114968151	22.3229428417
H129	5.1009876847	-0.7475661309	13.0407275435
H130	5.6945574696	-1.9106356301	14.2384098474

H131	3.5997877490	0.2697964030	14.6943536773
H132	3.3336330154	-1.4897957430	14.5698284296
C133	-2.6626305272	5.6680627623	20.4068698848
H134	-2.3905479198	6.5401918524	21.0012606505
H135	-3.6966026534	5.7797129606	20.0721365183
C136	-1.7483566555	5.6240359018	19.1870832247
H137	-2.0233939716	6.4408600396	18.5150754582
H138	-1.8452890251	4.6741367844	18.6540289128
C139	6.6551048097	6.1533553924	18.4395547022
H140	7.2540251198	6.4494518495	17.5817468993
H141	6.7393728881	6.9241273203	19.2082843808
C142	7.1980119925	4.8202943186	18.9576880416
H143	6.4331975829	4.2806531714	19.5224951395
H144	8.0399908129	5.0357624152	19.6239197319
C145	8.4494003277	2.9533926628	18.3006892950
H146	9.2969151541	3.3350230778	18.8787084128
H147	7.8724228725	2.2673856177	18.9297204861
C148	5.2768083716	-0.7593166276	20.2951111697
H149	6.3050066640	-0.7348466055	20.6335879377
C150	4.9937814172	-0.7500094283	18.9570685363
H151	5.7799418047	-0.6898406939	18.2181011392
C152	1.2344854775	-0.7606483243	19.0509110437
H153	0.4559431790	-0.7687179746	19.7978412019
C154	0.9389483435	-0.7283437145	17.7178830988
H155	-0.0906261893	-0.7077448791	17.3856696159
C156	1.9678470141	-0.7476053463	16.7397099685
H157	1.6943433228	-0.7294014874	15.6944219689

C158	1.4982058557	5.8565002623	16.4845341440
H159	1.3216374378	5.8121102955	15.4166348525
C160	-3.4222872188	3.4571328694	20.9874380091
H161	-4.4241922674	3.8377721985	20.7698671049
H162	-3.0732413800	2.8628513397	20.1376980545

1³⁺ CBPQT circling DNP (radical on the side)

-3759.269279 -3758.889415 -3759.912428 -3760.292292

N1	1.8261446986	9.2366701399	22.4422428625
C2	3.1694865601	9.2462910382	22.2168130625
C3	0.9772635100	9.2675283972	21.3765048941
C4	1.2826000850	8.9907670604	23.7951555511
C5	3.6890970409	9.2623555550	20.9561670635
C6	1.4322300783	9.2758695046	20.0947569053
C7	1.0172799086	7.4968146027	23.9378624276
C8	2.8359309221	9.2421703384	19.8050229286
C9	-0.2023434114	6.9541504727	23.5281140776
C10	2.0369613474	6.6406708177	24.3596561815
C11	3.3351695643	9.1961833647	18.4725120307
C12	-0.3717389717	5.5715101258	23.4492759191
C13	1.8682967923	5.2595287956	24.2906672766
C14	2.4711849648	9.1091004913	17.3326171810
C15	4.7361474003	9.2307333101	18.1665194235
C16	0.6793649169	4.7198027657	23.7944011233
C17	2.9764911072	9.0284853618	16.0706724738
C18	5.1765910425	9.1503779596	16.8791864084
C19	0.5624887932	3.2240510113	23.5509860427

N20	4.3167481046	9.0446911242	15.8269776186
N21	1.1393814133	2.9209289204	22.2032555737
C22	4.8222009443	8.7467882162	14.4695052107
C23	2.4176966407	2.5290386494	22.0915149994
C24	0.3856957117	3.1406440330	21.1136467000
C25	4.8899240158	7.2334571766	14.2950939731
C26	3.0022397932	2.3436360968	20.8525229173
C27	0.9192678677	2.9580269308	19.8490415847
C28	5.9530372929	6.5207626489	14.8549139035
C29	3.8489776509	6.5326194820	13.6831378412
C30	2.2544955522	2.5811718959	19.6947411262
C31	5.9348296114	5.1291775535	14.8904696139
C32	3.8356857795	5.1368892738	13.7012893942
C33	2.8898976665	2.5354170406	18.3387818175
C34	4.8559779559	4.4306766444	14.3418215898
C35	2.1275932121	2.4509070026	17.1718498236
C36	4.2793070538	2.6438621608	18.2062950589
C37	4.7426951619	2.9243966219	14.5291040520
C38	2.7582336014	2.5425376572	15.9410268583
C39	4.8598460205	2.6951303752	16.9555672512
N40	4.0905336112	2.6686020040	15.8526114581
O41	-0.4110878529	5.7291237645	19.6247864984
C42	0.5860120457	5.7927674390	18.7027510988
C43	1.9053117428	5.8775455834	19.2612698741
C44	0.3977497984	5.7293305625	17.3436344923
C45	3.0031240805	5.8664928677	18.3806504455
C46	2.1098138542	5.9440275968	20.6715233452

O47	-2.4896447513	4.5617763252	21.2426147129
C48	2.8003679555	5.8151346116	16.9733310952
C49	4.3286851675	5.9205587229	18.9321844114
C50	3.3857505857	5.9926409678	21.1547393954
O51	5.3247344083	5.8898800849	18.0112037938
C52	4.5133632926	5.9849939450	20.2891172282
C53	-3.3999175967	2.6503101980	22.3058944924
O54	-2.1384089518	1.9990185141	22.4142491704
C55	-2.1864157336	0.5956727354	22.2005724698
O56	7.5719046060	3.9979769744	17.9551883497
C57	-0.7712769690	0.0498081639	22.0918062283
O58	-0.0804973548	0.2125296978	23.3221637061
C59	8.9314162052	2.2123428682	17.1229025417
C60	0.7426708303	-0.8772355034	23.7080448368
O61	7.8788870139	1.4833763923	16.5144296266
C62	2.1144768689	-0.8405223318	23.0412698874
C63	8.3638679194	0.6539969222	15.4691545355
O64	1.8946674031	-0.8667007311	21.6378301840
C65	7.3619795456	-0.4394733801	15.1525188443
C66	2.9543243895	-0.8103374546	20.7928068332
O67	6.2619935544	0.0944603292	14.4303983402
C68	2.5978196360	-0.7737971769	19.4012588702
C69	4.2676288845	-0.7809641751	21.1832052046
C70	5.3231440755	-0.8999040481	14.0496983629
C71	3.6271177555	-0.7108459916	18.4422062487
C72	4.0101866594	-0.7235063161	14.7973316948
C73	3.2613127911	-0.7194902291	17.0535429825

O74	4.3041662634	-0.7015671259	16.1857922464
H75	3.8001636048	9.2410003967	23.0953906382
H76	-0.0780502099	9.2968042665	21.6089283952
H77	2.0155463403	9.3394491660	24.5194310054
H78	0.3681022037	9.5713869591	23.9014327273
H79	4.7643292606	9.2718386806	20.8679778816
H80	0.6918788994	9.3167996255	19.3104531391
H81	-1.0206070356	7.6088694160	23.2503685686
H82	2.9740033924	7.0487523423	24.7224389169
H83	-1.3064091716	5.1620692446	23.0803274980
H84	2.6745579904	4.6061604008	24.6051041834
H85	1.3980367769	9.0734271571	17.4334274807
H86	5.4824196453	9.3410978173	18.9388257761
H87	2.3366658268	8.9392438385	15.2032831139
H88	6.2285908299	9.1881058661	16.6315813341
H89	1.1260311690	2.6431680862	24.2760754959
H90	-0.4681517628	2.8768388884	23.5231965640
H91	4.1433511140	9.2004724151	13.7500214188
H92	5.8044571802	9.2051561883	14.3713232478
H93	2.9696048845	2.3948277848	23.0113768473
H94	-0.6301654624	3.4846508426	21.2773850950
H95	4.0322077756	2.0192774659	20.8236187640
H96	0.2903559280	3.1802815969	18.9991687404
H97	6.7948231764	7.0548179378	15.2800702200
H98	3.0362924457	7.0695277596	13.2068508972
H99	6.7484661933	4.5973564655	15.3723786105
H100	3.0160804321	4.6036494247	13.2324742278

H101	1.0548819151	2.3266034654	17.1805332203
H102	4.9326659073	2.7190515002	19.0620313690
H103	4.1178787734	2.4732647165	13.7618203416
H104	5.7046879551	2.4164689949	14.5542153592
H105	2.2051991493	2.5284734624	15.0113968352
H106	5.9315979477	2.7711077526	16.8179659632
H107	-0.5946551349	5.6607452235	16.9183656893
H108	1.2547060939	5.9725350929	21.3346877773
H109	3.6626595205	5.8404877743	16.3198420245
H110	3.5596710933	6.0481216720	22.2205528644
H111	5.5011546359	6.0369925913	20.7254658066
H112	-4.2103993411	1.9198414633	22.2722766175
H113	-3.5337063813	3.2876500592	23.1802764008
H114	-2.7115834782	0.1079840438	23.0261460694
H115	-2.7082280550	0.3745129192	21.2640751915
H116	-0.2384039311	0.5716697107	21.2947105524
H117	-0.8403846493	-1.0093662021	21.8319969370
H118	9.7257236238	1.5268743513	17.4335165464
H119	9.3488118493	2.9443461261	16.4252974484
H120	0.8849840258	-0.8100523390	24.7858456368
H121	0.2504186666	-1.8243660339	23.4747141334
H122	2.6489550283	0.0698396478	23.3175632242
H123	2.6966516167	-1.7102914230	23.3551505422
H124	8.5722507790	1.2456765058	14.5731464352
H125	9.2896213582	0.1668799233	15.7900531849
H126	7.0201644419	-0.9009419706	16.0804509138
H127	7.8677614151	-1.1948077580	14.5441947551

H128	4.5420850473	-0.8191616405	22.2289421809
H129	5.1264593471	-0.8182435007	12.9797927750
H130	5.7194623054	-1.8956945431	14.2554213840
H131	3.5220995692	0.2109056296	14.5117195683
H132	3.3511922259	-1.5602669083	14.5551164254
C133	-2.6375945537	5.7067089738	20.4162968933
H134	-2.3321220820	6.5695563626	21.0078380461
H135	-3.6801035325	5.8305894643	20.1164346600
C136	-1.7560833728	5.6480185002	19.1748353479
H137	-1.9898677420	6.4951054429	18.5257123891
H138	-1.9167306503	4.7172031880	18.6230693807
C139	6.6526401445	6.1524629664	18.4329901118
H140	7.1935240652	6.4624324745	17.5417824574
H141	6.6679866337	6.9677559077	19.1582948993
C142	7.3497419696	4.9238902703	19.0048268404
H143	6.7591920702	4.4594347291	19.7988685546
H144	8.3064423109	5.2476459487	19.4271029328
C145	8.4127519700	2.9277349662	18.3545305176
H146	9.2694872733	3.3158252156	18.9127661584
H147	7.8640492665	2.2233636247	18.9885183735
C148	5.2888272591	-0.6818346112	20.1941948116
H149	6.3198925045	-0.6405695747	20.5224750264
C150	4.9898796940	-0.6417249838	18.8605072041
H151	5.7664316056	-0.5422425575	18.1147796669
C152	1.2332346409	-0.8002231108	18.9939190014
H153	0.4632973681	-0.8612234554	19.7476305054
C154	0.9224378432	-0.7773830316	17.6627173358

H155	-0.1107888479	-0.8064363885	17.3416639099
C156	1.9414459588	-0.7473221895	16.6736413072
H157	1.6579449512	-0.7467876146	15.6303665951
C158	1.5269501331	5.7542371560	16.4784605475
H159	1.3607528934	5.7228547163	15.4087365037
C160	-3.4381243191	3.5189848614	21.0542526703
H161	-4.4403975331	3.9381210535	20.9351607186
H162	-3.1903996768	2.9220112085	20.1711838678

1²⁺ CBPQT circling DNP

-3759.403618 -3759.208178 -3760.237133 -3760.432572

N1	1.7996182612	9.2291117089	22.3763443320
C2	3.1435670458	9.2871244538	22.1630799791
C3	0.9620680594	9.2169368828	21.3016859149
C4	1.2529204954	8.9829592014	23.7288126977
C5	3.6750480196	9.3226598668	20.9078251289
C6	1.4292841940	9.2466800400	20.0245011702
C7	1.0302597575	7.4858312765	23.8999839504
C8	2.8354656461	9.2777388398	19.7472117573
C9	-0.1782590514	6.9024524848	23.5160641969
C10	2.0766561786	6.6631258910	24.3238544879
C11	3.3496837073	9.2595427155	18.4195272872
C12	-0.3097672705	5.5142041526	23.4628151587
C13	1.9443974824	5.2767866310	24.2784975050
C14	2.5029339062	9.1563241838	17.2685022525
C15	4.7515365468	9.3294951398	18.1269589323
C16	0.7667334609	4.6930868865	23.8042407514

C17	3.0273886594	9.0706263376	16.0150027523
C18	5.2126933787	9.2386259306	16.8481250123
C19	0.6929113631	3.1911956859	23.5569949808
N20	4.3700747761	9.1030637455	15.7870562363
N21	1.2372162844	2.8849046593	22.2183809430
C22	4.8947350967	8.7750837940	14.4438850667
C23	2.5402198203	2.5269721601	22.0514082475
C24	0.4580479540	3.0823796578	21.1180637920
C25	4.9196537950	7.2597742514	14.2791354221
C26	3.0939723466	2.3618777382	20.8164758303
C27	0.9498036227	2.9078534206	19.8592764765
C28	5.9217617336	6.5153638937	14.9073566518
C29	3.8972724106	6.5890920326	13.6080317634
C30	2.3228215658	2.5751584308	19.6282163160
C31	5.8654137056	5.1253834998	14.9348526389
C32	3.8505755210	5.1929556788	13.6144626150
C33	2.8885189338	2.5197938612	18.3230869217
C34	4.8133445650	4.4541350840	14.3038623027
C35	2.1038854716	2.6526138076	17.1317581688
C36	4.2951844868	2.3678700203	18.1010613214
C37	4.6716055502	2.9430099330	14.4546790775
C38	2.6986920654	2.7231451831	15.9097889429
C39	4.8352186056	2.4287796613	16.8517551702
N40	4.0510483524	2.6290482483	15.7554425408
O41	-0.4594126124	5.7963095280	19.6834661172
C42	0.5245926424	5.8525548866	18.7445912303
C43	1.8558517296	5.9226703358	19.2737782227

C44	0.3084926602	5.8288231683	17.3879342561
C45	2.9348994316	5.9352641592	18.3695105347
C46	2.0903367404	5.9600558937	20.6797728281
O47	-2.5365371075	4.5973627954	21.3558914464
C48	2.7014214361	5.9127966400	16.9668595378
C49	4.2712514734	5.9854003243	18.8946162686
C50	3.3745389268	6.0079866611	21.1372911727
O51	5.2557352425	6.0023442826	17.9577501191
C52	4.4829809007	6.0238528442	20.2485009964
C53	-3.4149767662	2.6580282217	22.4084286848
O54	-2.1762463292	1.9826766332	22.5816504602
C55	-2.2032655394	0.6338630449	22.1404763523
O56	7.6518501429	4.0643585356	17.8823223881
C57	-0.7957303916	0.0582994175	22.1145793973
O58	-0.2485134024	0.0438224868	23.4252555892
C59	9.0073870539	2.2339871183	17.1396313024
C60	0.6316580025	-1.0323856624	23.6970462037
O61	7.9778526879	1.4580162998	16.5560501377
C62	2.0076421731	-0.8865921638	23.0532998703
C63	8.4669029050	0.5887240603	15.5514911307
O64	1.8316242851	-0.9508016701	21.6462881198
C65	7.4269849601	-0.4702785649	15.2373844251
C66	2.9152268466	-0.8929635786	20.8294150460
O67	6.3689940859	0.0980196168	14.4816386685
C68	2.5945735821	-0.8010408642	19.4329947619
C69	4.2187794795	-0.9333114137	21.2504374360
C70	5.3916435827	-0.8534836596	14.0920477247

C71	3.6461768050	-0.7898867151	18.4971989924
C72	4.0930061860	-0.6749754377	14.8633110643
C73	3.3125723361	-0.7395344944	17.1012812897
O74	4.3700940164	-0.8021463894	16.2486609774
H75	3.7656221714	9.3040714921	23.0476293849
H76	-0.0956227769	9.1888515791	21.5223293271
H77	1.9691911383	9.3680255076	24.4515376914
H78	0.3208261968	9.5382486686	23.8193965076
H79	4.7504097361	9.3671344587	20.8305265876
H80	0.6955101587	9.2416506107	19.2329907750
H81	-1.0161097451	7.5300753860	23.2331395134
H82	3.0078282743	7.1026193638	24.6652387111
H83	-1.2346433561	5.0755010131	23.1037900857
H84	2.7740438503	4.6501075246	24.5871506450
H85	1.4294303218	9.0994280911	17.3555743381
H86	5.4858486878	9.4545212173	18.9085636223
H87	2.4010450225	8.9581366362	15.1413760440
H88	6.2677596898	9.2859986738	16.6158741866
H89	1.2814779533	2.6391201674	24.2872219085
H90	-0.3329263344	2.8283351389	23.5741873589
H91	4.2493766635	9.2464086207	13.7048639383
H92	5.8934810435	9.2010987202	14.3674705499
H93	3.1148097419	2.3919919608	22.9580367019
H94	-0.5616109040	3.3960020225	21.3067654862
H95	4.1304429201	2.0630957272	20.7726542096
H96	0.2761852428	3.0923946773	19.0357177401
H97	6.7430281040	7.0281817572	15.3943145171

H98	3.1269883562	7.1495655283	13.0898801329
H99	6.6207906884	4.5685850116	15.4800688056
H100	3.0466421665	4.6834717697	13.0947299589
H101	1.0267269078	2.7180497600	17.1631856338
H102	4.9759805241	2.2022221774	18.9217052763
H103	4.0354691753	2.5385925250	13.6679659129
H104	5.6338303044	2.4338145841	14.4265129011
H105	2.1279575696	2.8587856929	15.0007844318
H106	5.8983224062	2.3143024525	16.6737967124
H107	-0.6928995120	5.7715192533	16.9826974147
H108	1.2487617263	5.9506402143	21.3593693326
H109	3.5491438292	5.9263295357	16.2933426919
H110	3.5690944199	6.0337619507	22.2004200966
H111	5.4797290150	6.0652349165	20.6660621541
H112	-4.2395995594	1.9419498407	22.3753550298
H113	-3.5563750142	3.3185230304	23.2636881178
H114	-2.8349603849	0.0397996704	22.8074689624
H115	-2.6083635705	0.5730724579	21.1251955455
H116	-0.1624197081	0.6457301177	21.4494737990
H117	-0.8681876819	-0.9626955839	21.7280378247
H118	9.8122496615	1.5791711951	17.4882262323
H119	9.4179155298	2.9444308539	16.4162022879
H120	0.7679318041	-1.0642453826	24.7774499850
H121	0.1862967157	-1.9765756420	23.3702168034
H122	2.4638845939	0.0661560370	23.3272552827
H123	2.6410741852	-1.7087642456	23.3963616648
H124	8.7202684908	1.1464769244	14.6452027802

H125	9.3656959014	0.0781501887	15.9118457532
H126	7.0458388539	-0.8909662234	16.1687482871
H127	7.9100826886	-1.2618979988	14.6569324577
H128	4.4657430678	-0.9916094705	22.3018965210
H129	5.1755275454	-0.7190368722	13.0307879665
H130	5.7653220971	-1.8685366317	14.2434300738
H131	3.6622516760	0.3092094624	14.6705247909
H132	3.3908791773	-1.4481654806	14.5401550901
C133	-2.6870923144	5.7068128305	20.4867070119
H134	-2.3998609237	6.5931539463	21.0522144902
H135	-3.7296969117	5.8071576556	20.1747280484
C136	-1.7984682000	5.6350995345	19.2496306066
H137	-2.0801048149	6.4460731076	18.5727008271
H138	-1.9166883518	4.6796963669	18.7299264234
C139	6.5889150892	6.1515872914	18.4062435690
H140	7.1735471111	6.4439993932	17.5372559002
H141	6.6461764767	6.9480977683	19.1505694328
C142	7.1853890160	4.8568327419	18.9591297020
H143	6.4396592590	4.3042285990	19.5366273304
H144	8.0219523930	5.1158154687	19.6174236433
C145	8.4496702440	2.9861805370	18.3332243280
H146	9.2829903435	3.3653815871	18.9334802416
H147	7.8591426364	2.2961095068	18.9452013084
C148	5.2653465973	-0.8800680386	20.2862774818
H149	6.2899077156	-0.8942079711	20.6368073733
C150	4.9993065882	-0.8147868188	18.9463210894
H151	5.7956991110	-0.7523138690	18.2186364724

C152	1.2417472094	-0.7065106354	18.9986646013
H153	0.4549713895	-0.7030429094	19.7371067824
C154	0.9645950210	-0.6178145145	17.6643680731
H155	-0.0593303078	-0.5416998704	17.3219314135
C156	2.0044067643	-0.6489137994	16.6969389883
H157	1.7448470291	-0.5900118418	15.6495458168
C158	1.4179988976	5.8710119054	16.4995177622
H159	1.2316099703	5.8518840691	15.4322051725
C160	-3.4199628782	3.5071598344	21.1397094699
H161	-4.4346191339	3.8751460812	20.9619681861
H162	-3.1028303697	2.9107520752	20.2791451530

1⁺ CBPQT circling DNP (radical sandwiched by two DNP units)

-3759.517196 -3759.427362 -3760.466030 -3760.555865

N1	1.7606967594	9.3434959343	22.4567685315
C2	3.1289272074	9.3228305616	22.2295338565
C3	0.9414990343	9.2393464335	21.3409306937
C4	1.2234642723	8.9920071270	23.7712965179
C5	3.6715899126	9.2827419560	21.0001673475
C6	1.4113333000	9.1860474596	20.0840595800
C7	1.0297030632	7.4838796907	23.9013789307
C8	2.8519186739	9.2043129010	19.7792945763
C9	-0.1629140951	6.8880070326	23.4853361023
C10	2.0743164088	6.6635839984	24.3346004593
C11	3.3567877830	9.1717599726	18.5122390392
C12	-0.2830978709	5.5000630010	23.4178059162
C13	1.9558410612	5.2759344840	24.2752792239

C14	2.5230408853	9.0855725328	17.3033610745
C15	4.7916216260	9.2160892519	18.1826763440
C16	0.7917556964	4.6848168909	23.7782076542
C17	3.0439153559	9.0867430448	16.0663461014
C18	5.2411536930	9.2095301364	16.9141534242
C19	0.7276670681	3.1839983693	23.5321038978
N20	4.4029659779	9.2022088971	15.8097352208
N21	1.2734502056	2.8784509778	22.1945856963
C22	4.9102706175	8.8125695978	14.4933363786
C23	2.5861290621	2.5600659254	22.0253615987
C24	0.4869636673	3.0545631590	21.0961260133
C25	4.9184473901	7.2953152220	14.3183503679
C26	3.1400848248	2.4015907814	20.7900631319
C27	0.9778721960	2.8835060560	19.8371873075
C28	5.9179488075	6.5356334586	14.9316555240
C29	3.8960841363	6.6322187672	13.6378846028
C30	2.3569883090	2.5783331829	19.6040164834
C31	5.8625494797	5.1454490883	14.9346749749
C32	3.8470747908	5.2360424846	13.6196431169
C33	2.9167033725	2.5178390383	18.2970338237
C34	4.8114553873	4.4844302261	14.2924610733
C35	2.1235240323	2.6354555340	17.1106705678
C36	4.3236278363	2.3806869802	18.0664056459
C37	4.6715442233	2.9716549077	14.4215842582
C38	2.7095063507	2.7158674594	15.8852560917
C39	4.8540908886	2.4458482101	16.8134449889
N40	4.0613701598	2.6377239030	15.7221599864

O41	-0.4762621751	5.7613323547	19.6347661111
C42	0.5100767005	5.8201078554	18.6962010154
C43	1.8386846612	5.8920694863	19.2280511099
C44	0.2942073681	5.7878191183	17.3398125823
C45	2.9189241452	5.8901890001	18.3268354226
C46	2.0684563320	5.9499165714	20.6328729543
O47	-2.5489668437	4.5976394047	21.3109881823
C48	2.6866988021	5.8747189634	16.9248114175
C49	4.2534696516	5.9229049954	18.8558073151
C50	3.3501835171	5.9947037090	21.0937111312
O51	5.2441375047	5.8976063640	17.9251707812
C52	4.4609625152	5.9767300376	20.2089296825
C53	-3.4345842768	2.6579339241	22.3489142986
O54	-2.1945965853	1.9952893682	22.5605477177
C55	-2.2077475251	0.6349305334	22.1553150361
O56	7.6671701107	4.0366871638	17.8701564668
C57	-0.7953818229	0.0710289626	22.1439048283
O58	-0.2476895758	0.0926112112	23.4541840035
C59	9.0209279364	2.2140704548	17.1195270390
C60	0.6586503139	-0.9565037150	23.7453938569
O61	7.9801072786	1.4330410736	16.5637561146
C62	2.0279952952	-0.8000554413	23.0896730227
C63	8.4449773961	0.5704743978	15.5429237574
O64	1.8472780084	-0.9093385796	21.6862800562
C65	7.3903963055	-0.4760830734	15.2348618059
C66	2.9243740376	-0.8487327439	20.8604621034
O67	6.3317930222	0.1065869350	14.4911820480

C68	2.5915463157	-0.7833086306	19.4654183148
C69	4.2312172099	-0.8605704314	21.2716616546
C70	5.3449017066	-0.8338800544	14.1004911486
C71	3.6352280146	-0.7679002719	18.5207181009
C72	4.0529002918	-0.6579118770	14.8838203170
C73	3.2894065791	-0.7392532578	17.1273962695
O74	4.3402274108	-0.7973747511	16.2661376406
H75	3.7425787892	9.3682671346	23.1205500655
H76	-0.1201087975	9.2243969805	21.5501272432
H77	1.9183464874	9.3560473822	24.5281656583
H78	0.2701070353	9.5059386097	23.9014180546
H79	4.7497276247	9.2972530168	20.9340536970
H80	0.6842616388	9.1212465462	19.2885561018
H81	-0.9995790210	7.5111194403	23.1895266448
H82	2.9942516532	7.1081263864	24.6995821641
H83	-1.1977022958	5.0568523332	23.0377960359
H84	2.7845018644	4.6533650600	24.5955783416
H85	1.4522815098	8.9744355726	17.3851052490
H86	5.5312742367	9.2606405422	18.9694328324
H87	2.4185185850	8.9952880459	15.1880548655
H88	6.2995370933	9.2488695284	16.6883123949
H89	1.3178243191	2.6349182810	24.2635805715
H90	-0.2962013460	2.8152524198	23.5490548282
H91	4.2796111551	9.2746389301	13.7329106065
H92	5.9200132067	9.2115479858	14.3913371819
H93	3.1683067831	2.4533886142	22.9310772220
H94	-0.5377046722	3.3497943156	21.2868920457

H95	4.1862717072	2.1399101200	20.7442994199
H96	0.2984748570	3.0533725671	19.0153100275
H97	6.7365419554	7.0414371015	15.4293227497
H98	3.1244350477	7.2015704541	13.1310056444
H99	6.6169049744	4.5794828207	15.4717595261
H100	3.0402369508	4.7355064567	13.0951301514
H101	1.0468495339	2.6954906243	17.1521582720
H102	5.0126896167	2.2276783199	18.8824002150
H103	4.0307040580	2.5754217468	13.6342169485
H104	5.6341935009	2.4643440024	14.3808063880
H105	2.1319966587	2.8520095390	14.9806047176
H106	5.9173965292	2.3444905404	16.6309644148
H107	-0.7077756447	5.7280799713	16.9356901128
H108	1.2251936653	5.9761904386	21.3089573353
H109	3.5356559412	5.9035907297	16.2549145759
H110	3.5383095648	6.0536718833	22.1564384435
H111	5.4575873329	6.0143853104	20.6273390747
H112	-4.2514563066	1.9339484949	22.3002838977
H113	-3.6047398119	3.3260757453	23.1929028255
H114	-2.8349391429	0.0526610394	22.8368712368
H115	-2.6107601686	0.5440669385	21.1415585550
H116	-0.1678246127	0.6481341978	21.4646778167
H117	-0.8594789074	-0.9598729681	21.7829074473
H118	9.8353201508	1.5634206016	17.4536679908
H119	9.4127284368	2.9208603570	16.3821388581
H120	0.8028394664	-0.9567711164	24.8253471255
H121	0.2316747600	-1.9183164692	23.4458256664

H122	2.4661673969	0.1690369250	23.3334828677
H123	2.6795337096	-1.5984101272	23.4542754488
H124	8.6873319296	1.1351251478	14.6376819864
H125	9.3459755100	0.0494099218	15.8825475514
H126	7.0135043368	-0.8966562584	16.1680760651
H127	7.8591417792	-1.2706326733	14.6466205081
H128	4.4872124363	-0.8953624993	22.3221373924
H129	5.1199656149	-0.6860073117	13.0428031400
H130	5.7140065720	-1.8527894334	14.2365840725
H131	3.6223052139	0.3283874329	14.7029849116
H132	3.3481903552	-1.4280108772	14.5588131663
C133	-2.6959406926	5.7086146240	20.4426520875
H134	-2.3934866922	6.5904774419	21.0069797005
H135	-3.7405925782	5.8191663908	20.1400757294
C136	-1.8149149614	5.6283673254	19.2012245008
H137	-2.0843254335	6.4484125128	18.5296737708
H138	-1.9539825142	4.6787522958	18.6754475167
C139	6.5664130529	6.1052842509	18.3732874014
H140	7.1454705605	6.4070456640	17.5037130851
H141	6.5933817783	6.9128363982	19.1063278574
C142	7.2063922019	4.8395298115	18.9423168013
H143	6.4861560322	4.2818587993	19.5465370152
H144	8.0517792749	5.1305642960	19.5761573256
C145	8.4858275757	2.9745890551	18.3182509934
H146	9.3295301116	3.3699651030	18.8933296044
H147	7.9170058844	2.2870164546	18.9529488822
C148	5.2691153866	-0.8024552156	20.2982436515

H149	6.2963689162	-0.7904193257	20.6408405219
C150	4.9920397272	-0.7613866673	18.9596024948
H151	5.7813272441	-0.6897572364	18.2249574751
C152	1.2342589964	-0.7125804195	19.0414182685
H153	0.4539596076	-0.7098725015	19.7864819927
C154	0.9447642430	-0.6417563526	17.7086604205
H155	-0.0830882095	-0.5797106828	17.3746710794
C156	1.9768367114	-0.6706309354	16.7331213973
H157	1.7083424506	-0.6247868999	15.6873078068
C158	1.4049633260	5.8329630464	16.4536214242
H159	1.2224817863	5.8232122938	15.3854493745
C160	-3.4121839186	3.4974328655	21.0740172182
H161	-4.4256585434	3.8520427659	20.8637511951
H162	-3.0633339164	2.8981215849	20.2274620675

1¹⁺ CBPQT circling DNP (radical on the side)

-3759.501530 -3759.410095 -3760.449638 -3760.541073

N1	1.7933352820	9.2324558401	22.5005931498
C2	3.1327478036	9.2967117293	22.2618677949
C3	0.9373013429	9.2178540000	21.4405574166
C4	1.2725471677	8.9646136104	23.8604733693
C5	3.6411581137	9.3416638362	20.9974013522
C6	1.3808603004	9.2564969710	20.1554197032
C7	1.0536985383	7.4656930230	24.0131399016
C8	2.7809168996	9.2979955989	19.8520154775
C9	-0.1564290866	6.8871642809	23.6277224942
C10	2.1085599790	6.6366206071	24.4007715779

C11	3.2678053772	9.2824652594	18.5143460490
C12	-0.2813771785	5.5007407351	23.5358988635
C13	1.9803102958	5.2514123425	24.3180480714
C14	2.3978114931	9.1676729331	17.3821880709
C15	4.6624790647	9.3601611878	18.1906690045
C16	0.8019796077	4.6725104357	23.8383527908
C17	2.8968425793	9.0676102292	16.1190690128
C18	5.0970753659	9.2593962821	16.9038528255
C19	0.7269520548	3.1749793026	23.5437346950
N20	4.2336541730	9.1052418325	15.8621163743
N21	1.2490066297	2.8612384457	22.2195190208
C22	4.7344060351	8.7640305250	14.5130985520
C23	2.5785039925	2.5379218735	22.0237689420
C24	0.4763966888	3.0919624222	21.0930227966
C25	4.7840427805	7.2490646732	14.3564931302
C26	3.1294218768	2.3995351264	20.8038194195
C27	0.9542410899	2.9500040243	19.8431855835
C28	5.7817072890	6.5218483385	15.0109542246
C29	3.7993233015	6.5583288958	13.6518539690
C30	2.3621486550	2.6200819822	19.5700590572
C31	5.7639414395	5.1308884893	15.0208119494
C32	3.7979524107	5.1609823678	13.6359909759
C33	2.9037255918	2.5444255026	18.3212446626
C34	4.7610623615	4.4340191480	14.3390522388
C35	2.1355649582	2.7527443009	17.0880712423
C36	4.3231756693	2.2698555879	18.0504523209
C37	4.6803243221	2.9104161234	14.4345464052

C38	2.7092588072	2.7377813298	15.8763349832
C39	4.8396356056	2.2677938199	16.8091181539
N40	4.0591901177	2.4778391387	15.6785711762
O41	-0.5465625799	5.9670174000	19.8409141310
C42	0.4197879002	5.9753559477	18.8800734935
C43	1.7662623590	6.0018306673	19.3692193865
C44	0.1647556614	5.9594236566	17.5295134198
C45	2.8173547836	5.9902954014	18.4334032513
C46	2.0455912188	6.0151518966	20.7669892783
O47	-2.6313437936	4.6798214240	21.5177940019
C48	2.5434297629	5.9583407492	17.0396383520
C49	4.1687484142	6.0156373609	18.9186904140
C50	3.3418267605	6.0267688416	21.1864459825
O51	5.1292887125	6.0411503462	17.9557111670
C52	4.4230385120	6.0334712211	20.2646237604
C53	-3.4688913209	2.6420957864	22.4108513465
O54	-2.2337052459	1.9759762183	22.6234221662
C55	-2.1852622450	0.6888950429	22.0289842672
O56	7.6458782973	4.0296465063	17.8814957243
C57	-0.7760634275	0.1183613941	22.0830935554
O58	-0.3600556970	-0.0337319147	23.4337874017
C59	9.0160601400	2.1647703934	17.2303494478
C60	0.5961072017	-1.0552194900	23.6457471182
O61	8.0446126329	1.3667354475	16.5860814279
C62	1.9716091371	-0.7925545548	23.0336146300
C63	8.5935806628	0.4642822331	15.6481970282
O64	1.8458051720	-0.8800419930	21.6238969551

C65	7.5566581289	-0.5913728581	15.3080276147
C66	2.9526183744	-0.8337404162	20.8360824740
O67	6.5611009565	-0.0329577776	14.4672929616
C68	2.6665808498	-0.7532516575	19.4321951318
C69	4.2452585165	-0.9010103215	21.2876972836
C70	5.5428442927	-0.9562278274	14.1211537066
C71	3.7361898221	-0.7960985427	18.5189732999
C72	4.2551413699	-0.7204986191	14.8954512504
C73	3.4344195200	-0.7650440513	17.1152641576
O74	4.5038023423	-0.8953162270	16.2818166161
H75	3.7708980941	9.3086131956	23.1349169947
H76	-0.1157515881	9.1751951342	21.6798280202
H77	2.0032466635	9.3409210785	24.5736022842
H78	0.3426515627	9.5192513436	23.9770545165
H79	4.7146954603	9.3872356800	20.9000629626
H80	0.6335092721	9.2413046654	19.3769426412
H81	-0.9990114840	7.5194989868	23.3694700199
H82	3.0426369117	7.0721629807	24.7402872753
H83	-1.2065178477	5.0665069804	23.1720485317
H84	2.8167977183	4.6194048131	24.5965944118
H85	1.3268125838	9.0986417184	17.4926031480
H86	5.4125283619	9.4962630422	18.9545698879
H87	2.2533498474	8.9338531672	15.2609428398
H88	6.1466636732	9.3117484997	16.6491229138
H89	1.3082232442	2.6156260694	24.2775374735
H90	-0.3061635937	2.8317267556	23.5818824165
H91	4.0668166555	9.2172523105	13.7822497432

H92	5.7239228138	9.2065853356	14.4112688589
H93	3.1541515202	2.3897278261	22.9297546945
H94	-0.5460377325	3.3885408090	21.2940186450
H95	4.1686464290	2.1100568771	20.7542997397
H96	0.2701802554	3.1391330567	19.0289260834
H97	6.5685048195	7.0516384520	15.5349048854
H98	3.0273472030	7.1044053108	13.1202044374
H99	6.5108569877	4.5834268039	15.5874937101
H100	3.0276417676	4.6362756329	13.0810570602
H101	1.0736103222	2.9432434239	17.1359179556
H102	4.9928087048	2.0206638469	18.8611076691
H103	4.0932691969	2.5269308692	13.5962000511
H104	5.6726825138	2.4616485923	14.3941548631
H105	2.1403782149	2.9128003711	14.9709393838
H106	5.8846854918	2.0532607118	16.6185388150
H107	-0.8494929860	5.9339134578	17.1543235903
H108	1.2255158638	5.9952016754	21.4704109785
H109	3.3705715713	5.9202270082	16.3429556028
H110	3.5659765609	6.0218931379	22.2441650855
H111	5.4342307278	6.0406580540	20.6489962295
H112	-4.2785987926	1.9158349164	22.3004266599
H113	-3.6664299730	3.2572053453	23.2887292405
H114	-2.8774880537	0.0195187298	22.5497460024
H115	-2.4773538825	0.7430354156	20.9751521919
H116	-0.0832341177	0.7631135572	21.5438870585
H117	-0.8109398026	-0.8618029568	21.5959342004
H118	9.8070378997	1.5278974212	17.6399821692

H119	9.4656014210	2.8786023365	16.5333732116
H120	0.7216113638	-1.1444987446	24.7246329210
H121	0.2231045879	-2.0073479929	23.2547030838
H122	2.3447326768	0.1938956594	23.3116600216
H123	2.6531108109	-1.5639860889	23.4027361396
H124	8.9095667964	0.9863447654	14.7399606854
H125	9.4621514861	-0.0423897658	16.0822811544
H126	7.1101367129	-0.9630316158	16.2306402393
H127	8.0560158567	-1.4165274743	14.7902296648
H128	4.4671245864	-0.9422208210	22.3455938065
H129	5.3159715524	-0.8324036356	13.0606283677
H130	5.8861908812	-1.9814707561	14.2819991867
H131	3.8857906362	0.2928316136	14.7312227578
H132	3.5183825084	-1.4504366129	14.5476192151
C133	-2.7667563953	5.8074108890	20.6729946957
H134	-2.4726524257	6.6771131307	21.2607284082
H135	-3.8098068266	5.9245971623	20.3649431267
C136	-1.8844014957	5.7648341958	19.4297199115
H137	-2.2026501478	6.5692827851	18.7599814681
H138	-1.9804352050	4.8092240464	18.9060524093
C139	6.4744133487	6.0718064128	18.3849128015
H140	7.0727956819	6.3224523412	17.5123694413
H141	6.6062186450	6.8577416422	19.1313226822
C142	6.9642510718	4.7172345422	18.9176263692
H143	6.1137568107	4.1245004513	19.2627516713
H144	7.6526948530	4.8864720782	19.7536943070
C145	8.3551251704	2.9105800184	18.3782620995

H146	9.1258914195	3.2458392179	19.0807449417
H147	7.6794421581	2.2214355016	18.8945960178
C148	5.3127112749	-0.8921972513	20.3458587692
H149	6.3297359427	-0.9212333273	20.7179254517
C150	5.0769765104	-0.8482940430	18.9987947121
H151	5.8894444570	-0.8138428348	18.2869538724
C152	1.3271003519	-0.6203790878	18.9689845518
H153	0.5291743747	-0.5499895859	19.6919003032
C154	1.0820814690	-0.5528524945	17.6291208024
H155	0.0690141565	-0.4356773275	17.2649151073
C156	2.1393337868	-0.6379369191	16.6841867450
H157	1.9029027950	-0.5805500479	15.6318072214
C158	1.2471384273	5.9533251978	16.6092748302
H159	1.0315374016	5.9186304739	15.5477661232
C160	-3.4332728871	3.5576680913	21.1878955109
H161	-4.4537390280	3.8821548665	20.9606945009
H162	-3.0300403417	3.0253560508	20.3214638023

1⁰CBPQT circling DNP

-3759.603965 -3759.552467 -3760.600228 -3760.651725

C1	6.0672550828	10.5154485022	6.8900874181
C2	7.1486915595	10.5587093796	5.9060296160
C3	4.7754581064	10.2125835577	6.2742468111
C4	6.2533672010	10.7435417045	8.2332464645
C5	6.9437585586	10.3363454755	4.5944170718
C6	4.6331278756	10.0004913722	4.9510763679
C7	5.1775511915	10.7654773808	9.2233895044

C8	7.5547246523	11.0277461215	8.8358391344
N9	5.7052818467	9.9961892723	4.0633824871
C10	5.3996436487	10.9894908552	10.5348570846
C11	7.7152568088	11.2363977930	10.1560265121
N12	6.6705708641	11.1588072436	11.0715319688
C13	5.3082753369	11.6669542414	2.2756067703
C14	6.4182791977	12.4556182097	1.9636490819
C15	4.0537658442	12.2776606604	2.3538517581
C16	6.6882699847	13.2926331855	12.3383055053
C17	6.2896416819	13.8304988435	1.7824682854
C18	3.9218159430	13.6506504108	2.1643494383
C19	7.8016631173	14.1272705975	12.2186126935
C20	5.4161634992	13.8680954320	12.3104581452
C21	5.0410422806	14.4444872906	1.8990284727
C22	7.6388583963	15.5001033647	12.0292184976
C23	5.2501749840	15.2321500585	12.0968214653
C24	4.9262587918	15.9550515727	1.8544026038
C25	6.3626631441	16.0626489426	11.9382531969
N26	5.0346949529	16.5609476737	3.1749366638
C27	3.9449723218	16.5669903356	4.0417771376
C28	6.2955244562	16.6874596743	3.7501797921
N29	5.9319593704	17.7444284693	10.1677353024
C30	4.0657226057	16.7985877660	5.3627836588
C31	6.4718066608	16.9187604248	5.0627529603
C32	6.9955022288	17.6462146564	9.2834706016
C33	4.6581695949	17.5839856639	9.6369509269
C34	5.3588783541	17.0125831480	6.0065353038

C35	6.8359887629	17.4501838070	7.9619892231
C36	4.4437683480	17.3748626957	8.3212913107
C37	5.5275449153	17.2614616540	7.3476025194
O38	8.3014899458	13.6722792093	4.8573534857
C39	9.6763485585	13.5402019976	4.5766593687
C40	7.9478477435	13.9097853281	6.1553050368
C41	9.8293310066	12.8691642061	3.2257063429
C42	6.5485861767	13.8285639295	6.4283186383
C43	8.8478009749	14.1933120799	7.1619353829
O44	9.3840079039	13.6340690423	2.1266166360
C45	5.6031558625	13.5600828805	5.4043509158
C46	6.1169685631	14.0093887829	7.7635554945
C47	8.3841667984	14.3786778372	8.4845992661
C48	10.3354945005	14.5647996860	1.6519150913
C49	4.2765313001	13.4818640608	5.7177181828
C50	4.7195326272	13.8902044570	8.0528623806
C51	7.0524088969	14.2807279851	8.7872365411
C52	9.8111331498	15.1829668543	0.3664864070
C53	3.8164352193	13.6439600180	7.0464226636
O54	4.3955879326	14.0171491977	9.3695747959
O55	8.8208754333	16.1783520119	0.5480845168
C56	3.0905676585	13.6615264504	9.7622750891
C57	9.3469608028	17.4201829164	0.9846008596
C58	2.0918549509	14.8040023913	9.6493939887
C59	8.4364135688	18.5478388634	0.5549587629
O60	2.1751786279	15.6006891890	10.8150486718
O61	7.2526621900	18.5165144392	1.3168989502

C62	1.1118869708	16.5218134175	10.9186392095
C63	6.4095620826	19.6144951449	1.0501464512
C64	1.3102365520	17.3569127416	12.1646436222
C65	5.3779673131	19.7232259180	2.1470895172
O66	2.2445832912	18.3789085113	11.8879125527
O67	6.0557026232	20.0934790477	3.3364255663
C68	2.6732476011	19.0565485189	13.0486461841
C69	5.3298801322	20.1501521825	4.4840750984
C70	3.2933197883	20.3778695403	12.6557106317
C71	6.0946379758	20.3901001369	5.6722471822
C72	3.9627926420	20.0278098234	4.5438268227
O73	4.4115655404	20.1539682225	11.8281619689
C74	7.5066630424	20.5150645528	5.6326482625
C75	5.4069288610	20.5038849751	6.9050885682
C76	3.3035798928	20.1113113234	5.7940590061
C77	5.0743003802	21.3571703698	11.5132067156
C78	8.1975300128	20.7847345535	6.7871373406
C79	6.1652898233	20.7709186379	8.0879498184
C80	3.9976216115	20.3445678469	6.9505232057
C81	6.1071703371	21.1198842682	10.4371182178
C82	7.5327622922	20.9264469520	8.0271756245
O83	5.4254526485	20.8822769459	9.2209740781
H84	8.1593897962	10.8071995387	6.2101590186
H85	3.8784511146	10.1657728274	6.8826106788
H86	7.7517012095	10.3795980184	3.8702316583
H87	3.6672758799	9.7861460666	4.5016129126
H88	4.1474798180	10.6252792467	8.9140839911

H89	8.4369998415	11.1236434903	8.2127701097
H90	4.5884704035	11.0157806377	11.2574949427
H91	8.6834792835	11.4749408399	10.5869777506
H92	7.4035818042	12.0016613214	1.8772971662
H93	3.1748760307	11.6741811911	2.5773480652
H94	7.1755578901	14.4292237462	1.5835857875
H95	2.9391953054	14.1142005236	2.2396640348
H96	8.8027414170	13.6998362649	12.2588599768
H97	4.5434539998	13.2310492338	12.4418962193
H98	8.5153904687	16.1389196483	11.9282609964
H99	4.2478360792	15.6496681005	12.0078709243
H100	5.7278919577	16.3835698863	1.2415425725
H101	3.9643338904	16.2565148514	1.4221535609
H102	2.9822732488	16.4055358268	3.5630997499
H103	7.1211769101	16.6159855762	3.0494888162
H104	3.1560749245	16.8172526094	5.9548171264
H105	7.4938401109	17.0253498132	5.4067601140
H106	7.9772810034	17.7620833509	9.7363892028
H107	3.8495721894	17.6880373170	10.3547117863
H108	7.7334023520	17.4211819983	7.3552510782
H109	3.4111214103	17.3377137576	7.9882893503
H110	10.1613555031	12.8956641764	5.3245161630
H111	10.1761954368	14.5196725985	4.6062375177
H112	10.8831690729	12.5807274867	3.0883547826
H113	9.2251770074	11.9564101018	3.2335299224
H114	9.9085172656	14.2794825841	6.9499141189
H115	5.9470143033	13.4291176525	4.3853493843

H116	9.1011558335	14.6006689174	9.2724003093
H117	10.5458143317	15.3437933101	2.3998781046
H118	11.2853499707	14.0501250686	1.4343521342
H119	3.5516021456	13.2910667359	4.9317751471
H120	9.3515379382	14.3906448229	-0.2338061940
H121	10.6568522634	15.5990777806	-0.2015994319
H122	3.1564187201	13.3709923355	10.8147647036
H123	2.7464069618	12.7886167205	9.1944265583
H124	10.3379628060	17.5865506796	0.5362350353
H125	9.4583140828	17.4425294155	2.0771870020
H126	2.3051523127	15.4083703032	8.7561340804
H127	1.0746818172	14.3894801810	9.5567517671
H128	8.9629268071	19.5021894525	0.7141470648
H129	8.2180410872	18.4599676968	-0.5211587626
H130	1.0753703658	17.1823507893	10.0384505860
H131	0.1524271356	15.9842365310	10.9791537830
H132	6.9958140385	20.5455739014	1.0098666847
H133	5.9019314553	19.4942930037	0.0802164349
H134	0.3528401172	17.7979924738	12.4810112453
H135	1.6683045776	16.7069359507	12.9773066856
H136	4.6358450299	20.4869404862	1.8740689946
H137	4.8721212441	18.7617512600	2.2957064621
H138	1.8222411024	19.2620255321	13.7160128243
H139	3.3951862248	18.4396469183	13.6060963905
H140	3.5856776293	20.9163149389	13.5721443943
H141	2.5483451755	20.9932589743	12.1284110890
H142	3.3823864116	19.8326833595	3.6491877191

H143	8.0181088214	20.3911435401	4.6844033692
H144	2.2245032970	19.9816285930	5.8239309959
H145	4.3558742230	22.1104568214	11.1551542945
H146	5.5719517351	21.7678865553	12.4064787327
H147	9.2797677098	20.8876372278	6.7608936912
H148	6.7434576998	20.2600389540	10.6836688710
H149	6.7366203932	22.0166611786	10.3532969987
H150	6.6911424288	14.4148638149	9.7988222739
H151	2.7524779210	13.5773189169	7.2496602766
C152	5.4714034360	10.2032387864	2.6327097561
H153	6.3198672771	9.7687589035	2.0913188489
H154	4.5761147914	9.6339909539	2.3594575596
C155	6.8298905849	11.7841914007	12.3871488608
H156	6.0756728044	11.3488162951	13.0524689667
H157	7.8158849024	11.5008314730	12.7717936801
C158	6.1665225658	17.5255114867	11.5882242950
H159	5.3097052862	17.9467862249	12.1203743474
H160	7.0534720491	18.1041947665	11.8784244030
H161	3.4986646489	20.3813773766	7.9119345329
H162	8.1125009010	21.1210847090	8.9226687672

2⁴⁺ CBPQT circling glycol chain

-3759.049507 -3758.381699 -3759.403774 -3760.071581

N1	2.0092917280	18.6762784229	6.3749132439
C2	0.8253405058	17.7450592036	6.3457503846
C3	1.8645435573	19.9766045605	6.0740711214
C4	3.2049215691	18.1821810637	6.7375922835
C5	0.6439111729	17.1145812144	7.7173346001

C6	2.9320623509	20.8562443500	6.1796065619
C7	4.3100784868	19.0030040720	6.8332582736
C8	-0.1032953908	17.7489980936	8.7133389551
C9	1.2710234306	15.9025530830	7.9974955901
C10	4.1763638620	20.3724978037	6.5847573418
C11	-0.1591796198	17.1940332651	9.9886869602
C12	1.2519424649	15.3700745339	9.2862680822
C13	5.3300005133	21.2781783900	6.8832220296
C14	0.5542215151	16.0312301983	10.2930482098
C15	5.1099101862	22.4775726404	7.5705704414
C16	6.6424320816	20.9015382057	6.5967724995
C17	0.6089159336	15.5403041271	11.7344505677
C18	6.1930127230	23.1942688860	8.0388184361
C19	7.6885310552	21.6679949122	7.0870617175
N20	1.6345220677	16.3582537182	12.4599028136
N21	7.4476780661	22.7597220843	7.8278047410
C22	1.2810444261	17.5640385345	12.9370045309
C23	2.9085090844	15.9470635704	12.5079724249
C24	8.5647831173	23.4406688173	8.5586765387
C25	2.2248481582	18.4425747959	13.4309413123
C26	3.9007771989	16.7761788554	13.0085764488
C27	8.4523257641	23.0620581604	10.0325856019
C28	3.5696643120	18.0597817594	13.4500824292
C29	8.0585891471	24.0002387834	10.9808318776
C30	8.6915297376	21.7394869531	10.4292332203
C31	4.6348763429	19.0445966024	13.8238607320
C32	7.8668758278	23.6168970289	12.3137638081

C33	8.5017213379	21.3593605496	11.7503937622
C34	4.4124641437	20.4105555336	13.5945046279
C35	5.8823506300	18.6408255746	14.2977998222
C36	8.0701197417	22.2958297944	12.6993436834
C37	5.4566315987	21.2968420884	13.7553956233
C38	6.8922852004	19.5821907324	14.4400330926
C39	7.8031621020	21.8547540209	14.1347142487
N40	6.6749505986	20.8692105058	14.1367001884
O41	5.5378482305	15.2291443616	8.6207415896
C42	4.6662816018	14.1847883531	8.6253091301
C43	6.0555341481	15.7058179692	9.8531901614
C44	3.9263353584	14.0283751548	7.4073929413
C45	4.4875477892	13.3129485185	9.6701095463
C46	6.1038530867	17.2240096768	9.7806927098
C47	4.1813440066	14.8630888908	6.2807532471
C48	2.9409386568	13.0199813575	7.3393981478
C49	3.5066789117	12.2861737581	9.5683525356
O50	4.7673951653	17.6762140516	9.6378282202
C51	3.4462938753	14.6940537744	5.1382475090
C52	2.1723568340	12.8881876095	6.1286399827
C53	2.7354529410	12.1471132035	8.4463798866
C54	4.5105957264	18.9544389374	10.1739880513
C55	2.4268541510	13.7074828437	5.0528755476
O56	1.2290984057	11.9239044984	6.1508536303
C57	2.9955656532	19.1493158507	10.1475399807
C58	0.6063231843	11.5604887306	4.9189888060
O59	2.6757556299	20.2425295910	10.9792325996

C60	-0.4877925086	10.5407380534	5.2050850030
C61	1.3298216389	20.6683186548	10.8360218213
O62	-1.6534228499	11.2396338550	5.5941051629
C63	1.0855072348	21.8449830687	11.7675061643
O64	1.1282940137	21.4323389628	13.1304182419
C65	-0.0388051881	21.6965738625	13.9025457381
O66	-4.0112604625	11.9922176186	7.0911469823
C67	-1.0186733392	20.5327053364	13.8282905335
O68	-1.4460176364	20.4152426185	12.4765952692
C69	-2.1758398633	19.3237397810	12.1124103783
O70	-5.2280831854	14.7123408520	7.2763437933
C71	-2.4511865473	18.2616911643	12.9390531933
C72	-2.6486653290	19.3402532009	10.7543989097
C73	-3.1823474445	17.1468593818	12.4343666177
C74	-3.3921376897	18.2348517637	10.2897939609
C75	-2.3870756467	20.4437614567	9.8905475915
C76	-5.1321092148	17.1127116737	7.2606892463
C77	-3.6387738994	17.1227919690	11.1462941137
C78	-3.8890905219	18.2513215514	8.9402721926
C79	-2.8651348817	20.4178107916	8.6084285217
O80	-4.6263470044	17.1755825971	8.5905452144
C81	-3.6179429174	19.3172896382	8.1162910115
H82	-0.0330200776	18.3392524242	6.0444087915
H83	1.0329036287	16.9998493200	5.5796622314
H84	-0.3379420877	15.6783297750	12.2522497498
H85	0.9078558513	14.4977063244	11.8071116476
H86	9.4957497747	23.0966149188	8.1150786333

H87	8.4564320758	24.5111790165	8.4016478396
H88	7.5067471259	22.6898344252	14.7654173436
H89	8.6637285027	21.3543265246	14.5718944839
H90	5.3845101526	15.4362387731	10.6672390730
H91	7.0460448900	15.2889779209	10.0363912334
H92	6.7214276382	17.5559690176	8.9420121587
H93	6.5433220990	17.5988943900	10.7105941533
H94	4.8559791560	19.0124340568	11.2091712707
H95	5.0151168969	19.7418021763	9.6033622827
H96	2.5195739620	18.2274226021	10.4970555637
H97	2.6539453751	19.3359982921	9.1237647753
H98	0.1433897058	12.4302637485	4.4528524457
H99	1.3613156609	11.1397457746	4.2521341102
H100	-0.6778485424	9.9730695358	4.2886945241
H101	-0.1581539460	9.8496855598	5.9861095536
H102	1.1512863685	20.9849783255	9.8026542457
H103	0.6385032561	19.8573486926	11.0819974385
H104	1.8645512277	22.5913917285	11.6064330419
H105	0.1174125940	22.2858299328	11.5323299153
H106	0.2763934754	21.8153940224	14.9381191849
H107	-0.5174804470	22.6191360503	13.5695394850
H108	-0.5085628835	19.6220649747	14.1494585821
H109	-1.8758585027	20.7089315684	14.4813373397
H110	-4.3029533615	17.0657147877	6.5536102930
H111	-5.7438871995	17.9945008830	7.0555727491
H112	0.8853176362	20.3041895008	5.7540222078
H113	3.2493753452	17.1315567366	6.9888570622

H114	2.7679909307	21.8991957060	5.9428896484
H115	5.2439842592	18.5659566634	7.1575334922
H116	-0.6511776956	18.6626637180	8.5049161257
H117	1.7840608884	15.3670243991	7.2084813357
H118	-0.7689851711	17.6715016089	10.7474069758
H119	1.7683639569	14.4371119071	9.4862029530
H120	4.1147126789	22.8397507143	7.7898297909
H121	6.8748153802	20.0223174845	6.0109593123
H122	6.0828753720	24.1028892442	8.6151167897
H123	8.7239192204	21.4067386743	6.9151250220
H124	0.2275469912	17.8040257976	12.8909633835
H125	3.1144371095	14.9555340696	12.1286825419
H126	1.9014611922	19.4224563241	13.7586068957
H127	4.9176081529	16.4072363128	13.0209265779
H128	7.8918077794	25.0316883260	10.6924236111
H129	9.0351164966	21.0067519326	9.7075454306
H130	7.5537453470	24.3558378585	13.0420376970
H131	8.6995824620	20.3345224877	12.0448767810
H132	3.4602461409	20.7801311881	13.2348808195
H133	6.1017500285	17.6132979932	14.5542566577
H134	5.3590014152	22.3559677199	13.5590997549
H135	7.8836132211	19.3151913961	14.7796289831
H136	5.0986979426	13.3718297274	10.5608913690
H137	4.9771454274	15.5937125571	6.3363377873
H138	3.3809999611	11.6054806704	10.4005000454
H139	3.6437927745	15.3079542058	4.2681121542
H140	1.9823316386	11.3755014917	8.3730500908

H141	1.8712121644	13.6079312082	4.1315528218
H142	-2.1457642070	18.2613660954	13.9773043875
H143	-3.3808976843	16.3158178317	13.0990634542
H144	-1.8374066999	21.2949437295	10.2668883689
H145	-4.1916211350	16.2781760302	10.7598935899
H146	-2.6878053734	21.2563034338	7.9465721143
H147	-3.9815027169	19.3428228165	7.0987203669
C148	-6.0090001343	15.8785921351	7.1238305787
H149	-6.4670416339	15.9124046599	6.1296707662
H150	-6.8038832912	15.9085588111	7.8753513547
C151	-5.9501625114	13.5332605512	6.9624038912
H152	-6.9664060270	13.5963797686	7.3656371305
H153	-6.0204316899	13.4080425943	5.8768707566
C154	-4.0364432046	11.2488512188	5.8875111773
H155	-4.0939993868	11.9070038888	5.0168919331
H156	-4.8981964424	10.5740957246	5.8762530805
C157	-2.7749125238	10.3983879273	5.7900937152
H158	-2.8857404985	9.7169280557	4.9395800758
H159	-2.6567184686	9.8081391964	6.7034946453
C160	-5.2786644772	12.3311814113	7.6212954678
H161	-5.9565676303	11.4742451636	7.5523231586
H162	-5.1265745155	12.5732404845	8.6716271258

1³⁺ CBPQT circling glycol chain

-3759.202278 -3758.805587 -3759.830844 -3760.227536

N1	1.7015849865	18.7087980839	6.4405787264
C2	0.6337060647	17.6868320780	6.4996903649

C3	1.4490187242	19.9977674244	6.7956192820
C4	2.9828668941	18.3383326389	6.1660606308
C5	0.6003529666	17.0418694896	7.8811541906
C6	2.4471498357	20.9184899556	6.9275313956
C7	4.0281017948	19.2057969287	6.2781713705
C8	-0.3768157558	17.3808907999	8.8117794225
C9	1.5875093036	16.1180069517	8.2305525767
C10	3.8184538133	20.5574581986	6.7070815952
C11	-0.3531852814	16.8215645176	10.0914289881
C12	1.6265083085	15.5757583410	9.5078379803
C13	4.8978392821	21.4571062837	6.9371579875
C14	0.6602780593	15.9355454164	10.4492108638
C15	4.7168094756	22.7231698111	7.5862947523
C16	6.2523016193	21.1444648671	6.5815760254
C17	0.7829824239	15.4247789521	11.8772463956
C18	5.7900313203	23.4732475549	7.9576416019
C19	7.2835648655	21.9471922329	6.9690927596
N20	1.8201717288	16.2632005474	12.5640569586
N21	7.0711913163	23.0828236147	7.6929002240
C22	1.5123806204	17.5426733984	12.8375300033
C23	3.0579034405	15.7992489995	12.7711284723
C24	8.1744742973	23.7121256041	8.4338328618
C25	2.4639704182	18.4294618241	13.2933788010
C26	4.0630977414	16.6418259856	13.2257160935
C27	8.1929354842	23.1795623110	9.8712456114
C28	3.7825028382	17.9867080520	13.4722392512
C29	8.7009215311	23.9557246736	10.9150138178

C30	7.6777663871	21.9178746506	10.1668860481
C31	4.8714037946	18.9601428094	13.8178694036
C32	8.6633696952	23.4915086389	12.2306386098
C33	7.6512225930	21.4482277454	11.4750042629
C34	4.6275840211	20.3408200143	13.7643212660
C35	6.1693113039	18.5331869863	14.1091172360
C36	8.1259360676	22.2362166475	12.5226141268
C37	5.6798299163	21.2202137062	13.9140561915
C38	7.1902764869	19.4646061145	14.2242423499
C39	8.0530860600	21.7530762097	13.9728631642
N40	6.9371501154	20.7740204327	14.0932285128
O41	5.8819602041	14.8748365191	8.9291449755
C42	4.8329736249	14.0085242636	8.9453505823
C43	6.3598196909	15.4520177070	10.1398476691
C44	4.0724758362	13.9626121425	7.7305929753
C45	4.5325243096	13.1720130783	9.9923982753
C46	6.2234810528	16.9635629702	10.0468669213
C47	4.4198223068	14.7763699569	6.6108424898
C48	2.9801281517	13.0708713484	7.6522114047
C49	3.4209696371	12.2909477390	9.8936633851
O50	4.8467806150	17.2780051932	10.0553337887
C51	3.6973969838	14.6645304646	5.4535658812
C52	2.2319463539	12.9993357568	6.4243691083
C53	2.6537316190	12.2413710896	8.7612890102
C54	4.6031835854	18.6623493061	10.1773278594
C55	2.5927755766	13.7736682136	5.3485815200
O56	1.2078826380	12.1164318630	6.4236889462

C57	3.0950499479	18.8992829367	10.0862012500
C58	0.6512178586	11.7474154103	5.1634378592
O59	2.8034471533	20.0404637965	10.8713155573
C60	-0.4464430215	10.7127238122	5.3820061189
C61	1.4777842130	20.5067822493	10.7005401781
O62	-1.6448278036	11.3884427940	5.7046230668
C63	1.2628855889	21.7043916135	11.6144436301
O64	1.2435485454	21.3167802263	12.9879247843
C65	0.0486695438	21.6089255871	13.7045279406
O66	-4.1564776955	12.0296217417	7.0019102036
C67	-0.9583043307	20.4698988462	13.6028433560
O68	-1.3479128962	20.3511845168	12.2403220501
C69	-2.1827631926	19.3318386890	11.8897777099
O70	-5.3064064126	14.8004508786	7.0898925321
C71	-2.6090472781	18.3494797338	12.7493447521
C72	-2.6065751760	19.3417905518	10.5166617242
C73	-3.4598557079	17.3127015403	12.2692373170
C74	-3.4568319897	18.3069010665	10.0697833582
C75	-2.1978171449	20.3721961543	9.6209870219
C76	-5.1006146493	17.1934087216	6.9862226833
C77	-3.8728442249	17.2808517548	10.9663478926
C78	-3.8939812806	18.3128330730	8.6988844643
C79	-2.6328476533	20.3457206597	8.3241109827
O80	-4.7212028382	17.3020961628	8.3547348464
C81	-3.4802695047	19.3090417276	7.8452740990
H82	-0.3092675464	18.1780049657	6.2680698997
H83	0.8409160792	16.9472910718	5.7281064964

H84	-0.1423326493	15.5275836679	12.4399274338
H85	1.1206358381	14.3923630700	11.9214515969
H86	9.1024430199	23.4794986091	7.9144847160
H87	8.0292198862	24.7912413537	8.4279839223
H88	7.8501829663	22.5769661079	14.6540470549
H89	8.9646738392	21.2436916013	14.2780970916
H90	5.7753877399	15.1058072958	10.9893766334
H91	7.4030369718	15.1699950596	10.2743527602
H92	6.6964732028	17.3297398256	9.1317064158
H93	6.7277594012	17.4138065700	10.9107143884
H94	4.9476064911	19.0247760731	11.1524281470
H95	5.1271367649	19.2228095902	9.3949944149
H96	2.5739897817	18.0153308470	10.4661941238
H97	2.7890027827	19.0555723066	9.0482194154
H98	0.2080258428	12.6142974819	4.6706221527
H99	1.4436491497	11.3285030245	4.5392243467
H100	-0.5712010588	10.1524489158	4.4496067542
H101	-0.1535528351	10.0162637708	6.1733480025
H102	1.3265581468	20.8200401713	9.6625151514
H103	0.7507703349	19.7230289779	10.9365666478
H104	2.0836412842	22.4073554227	11.4698095118
H105	0.3254800300	22.1925850153	11.3490923144
H106	0.3206549541	21.7330371218	14.7516485628
H107	-0.3952774038	22.5379656836	13.3424704085
H108	-0.4879559097	19.5456250530	13.9470784157
H109	-1.8297098478	20.6809662436	14.2267117981
H110	-4.2086797613	17.0765384420	6.3695985795

H111	-5.6473327749	18.0894843548	6.6823799941
H112	0.4096161832	20.2453114177	6.9634529189
H113	3.1224874331	17.3111156850	5.8618768139
H114	2.1622870344	21.9286778294	7.1801263970
H115	5.0141306944	18.8284936707	6.0506781186
H116	-1.1671235754	18.0728437714	8.5479350883
H117	2.3372880778	15.8186387242	7.5085468433
H118	-1.1352112556	17.0770116115	10.7975954246
H119	2.4139484715	14.8774258439	9.7660302771
H120	3.7367291322	23.0960012681	7.8407307789
H121	6.4957165377	20.2717963951	5.9934160477
H122	5.6825716720	24.4008166288	8.5040118868
H123	8.3144345312	21.7137787024	6.7375070927
H124	0.4899152939	17.8371749473	12.6443953813
H125	3.2334603184	14.7537270214	12.5584935508
H126	2.1498787309	19.4544523515	13.4398211310
H127	5.0448278849	16.2135803072	13.3640800687
H128	9.1045344142	24.9412027428	10.7114418617
H129	7.2735382052	21.2897646748	9.3835624094
H130	9.0359934627	24.1221089976	13.0299365671
H131	7.2389882925	20.4628953989	11.6620274343
H132	3.6477533096	20.7517546622	13.5606712745
H133	6.4325036997	17.4931462315	14.2288694302
H134	5.5574454019	22.2920711626	13.8543466927
H135	8.2190473665	19.1738696362	14.3881090034
H136	5.1519470584	13.1466294022	10.8793773822
H137	5.2577840416	15.4547322347	6.6928691137

H138	3.1982827693	11.6394911805	10.7288928438
H139	3.9673711574	15.2513962382	4.5833077799
H140	1.8102117571	11.5702897627	8.6831709192
H141	2.0554331119	13.7134114832	4.4129112078
H142	-2.3237911500	18.3544211989	13.7925287690
H143	-3.7790617744	16.5431557834	12.9602592578
H144	-1.5688682401	21.1713671320	9.9862580089
H145	-4.5105168417	16.4907482129	10.5959598608
H146	-2.3461297690	21.1326198894	7.6375805998
H147	-3.8015215562	19.3287570619	6.8136950088
C148	-6.0127856286	15.9900693810	6.8138464419
H149	-6.3645566284	15.9994528652	5.7767093709
H150	-6.8796955601	16.0846967666	7.4752753570
C151	-6.0151312336	13.6477832487	6.6719398287
H152	-7.0704974654	13.7334160371	6.9537686725
H153	-5.9622153041	13.5450223979	5.5833508233
C154	-4.0447017401	11.4186496538	5.7323989430
H155	-3.9896751576	12.1652768070	4.9372809323
H156	-4.9066284377	10.7686763445	5.5485709744
C157	-2.7885698906	10.5550206080	5.6935017278
H158	-2.8108883351	9.9613932355	4.7732785432
H159	-2.7799324311	9.8758765960	6.5514187437
C160	-5.4659528472	12.4093926565	7.3774182366
H161	-6.1612543490	11.5809693029	7.2011680012
H162	-5.4319427429	12.6201815047	8.4452852872

1²⁺ CBPQT circling glycol chain

-3759.356822 -3759.156787 -3760.186610 -3760.386645

N1	1.6878946829	18.6923953995	6.4122039515
C2	0.6268353433	17.6631515228	6.4828099122
C3	1.4339154696	19.9742443578	6.7890154717
C4	2.9664561008	18.3347998607	6.1148617882
C5	0.6010548389	17.0268594234	7.8674975614
C6	2.4286934214	20.8978831372	6.9206722292
C7	4.0064460475	19.2087047916	6.2226860227
C8	-0.3732104939	17.3737766958	8.7977871018
C9	1.5934069366	16.1099111719	8.2224330859
C10	3.7995351726	20.5487292849	6.6858973617
C11	-0.3454921200	16.8201538511	10.0798053817
C12	1.6330919248	15.5738018927	9.5025890335
C13	4.8777534165	21.4448736222	6.9369088555
C14	0.6643823103	15.9324961409	10.4426151800
C15	4.6958805136	22.6963216404	7.6144490037
C16	6.2345748927	21.1415697270	6.5807801596
C17	0.7821162131	15.4240524432	11.8740435087
C18	5.7660777527	23.4475351165	7.9915128196
C19	7.2628159789	21.9453954138	6.9748887336
N20	1.7939804144	16.2375844089	12.5859837272
N21	7.0481121101	23.0735722787	7.7089340077
C22	1.5063021864	17.5433908541	12.8503268886
C23	3.0544248250	15.7854590814	12.8032877621
C24	8.1531639152	23.7107649426	8.4412930005
C25	2.4514908942	18.4254353390	13.2736210776
C26	4.0484506226	16.6112177070	13.2475787653

C27	8.1785347621	23.1891015258	9.8815420733
C28	3.8100823601	18.0078093783	13.4570385251
C29	8.6900778754	23.9726316241	10.9181462809
C30	7.6621548601	21.9292579788	10.1847285621
C31	4.8470300785	18.9347066845	13.7680080071
C32	8.6615522538	23.5117130810	12.2354118027
C33	7.6386313873	21.4680097885	11.4958957379
C34	4.6217612191	20.3528624864	13.7881018410
C35	6.2028074132	18.5338388156	14.0129021418
C36	8.1250222476	22.2582672162	12.5368310252
C37	5.6568775568	21.2205758422	13.9516199433
C38	7.1967406212	19.4557148246	14.1657613337
C39	8.0372452690	21.7695732025	13.9857894914
N40	6.9452853491	20.7928641889	14.1166142296
O41	5.8786837110	14.8464739263	8.9685837537
C42	4.8328917751	13.9771931910	8.9679518907
C43	6.2994120187	15.4531479016	10.1885452794
C44	4.0829754835	13.9280117279	7.7464917874
C45	4.5243868990	13.1409429708	10.0126948769
C46	6.2197708758	16.9642929169	10.0409270107
C47	4.4351706848	14.7477969820	6.6331066626
C48	2.9925680658	13.0359342735	7.6592672038
C49	3.4158408486	12.2578985564	9.9048548824
O50	4.8597253176	17.3120651686	9.9253483326
C51	3.7231294723	14.6389931604	5.4698802150
C52	2.2530721849	12.9696161645	6.4260283124
C53	2.6583484674	12.2059294182	8.7657801738

C54	4.6168814042	18.6870837960	10.1433088561
C55	2.6198300844	13.7471929062	5.3545859807
O56	1.2283207149	12.0868366975	6.4177181773
C57	3.1084047815	18.9159083467	10.0665692240
C58	0.6663503600	11.7350648011	5.1563897304
O59	2.8272479531	20.0966733323	10.7940873139
C60	-0.4429437905	10.7118536014	5.3675489586
C61	1.4769016543	20.4998089502	10.6954019476
O62	-1.6363968708	11.3933185240	5.6979398065
C63	1.2610072404	21.7146137223	11.5905482684
O64	1.2645686398	21.3658031838	12.9730634732
C65	0.0712119762	21.6223266081	13.6973068328
O66	-4.1543984648	12.0360904835	6.9993662857
C67	-0.9118118506	20.4610349117	13.6108783068
O68	-1.3390311745	20.3571420182	12.2587356324
C69	-2.1732270412	19.3389154586	11.9119098646
O70	-5.2904279440	14.8151664104	7.1014048059
C71	-2.5909647570	18.3503449765	12.7678979458
C72	-2.6079875474	19.3577378647	10.5425069909
C73	-3.4484522826	17.3198187347	12.2870964408
C74	-3.4639376384	18.3299744039	10.0950875688
C75	-2.1933198828	20.3870937670	9.6485652527
C76	-5.0871474294	17.2122262509	7.0051037910
C77	-3.8748919895	17.2986240835	10.9883017114
C78	-3.8997510301	18.3395937692	8.7240406072
C79	-2.6286216305	20.3659125330	8.3519400719
O80	-4.7278067758	17.3289567288	8.3773518515

C81	-3.4813972029	19.3338047290	7.8714072598
H82	-0.3201540045	18.1466818987	6.2507182366
H83	0.8392697948	16.9229176902	5.7136000320
H84	-0.1624062503	15.5125205087	12.4091296764
H85	1.1104001956	14.3871875510	11.9038894902
H86	9.0789613628	23.4771150897	7.9177501936
H87	8.0049529236	24.7893382075	8.4275300390
H88	7.8420810825	22.6047265191	14.6572749747
H89	8.9605424198	21.2801988920	14.2928341344
H90	5.6423987414	15.1614669012	11.0035740047
H91	7.3196168966	15.1392063513	10.4029775909
H92	6.7856784970	17.2942553377	9.1649567171
H93	6.6608677737	17.4180413152	10.9366903197
H94	4.9524166554	18.9782067646	11.1432573507
H95	5.1392132870	19.2993943420	9.3989982549
H96	2.6036164574	18.0539523445	10.5091985623
H97	2.7833703685	19.0137366872	9.0262310315
H98	0.2369392696	12.6101553577	4.6708391408
H99	1.4514936206	11.3145100676	4.5247504987
H100	-0.5742853302	10.1596744938	4.4315536473
H101	-0.1548578460	10.0080447941	6.1535255910
H102	1.2466412161	20.7777073918	9.6613455313
H103	0.8005014663	19.6938180028	10.9942435682
H104	2.0754412079	22.4194683570	11.4181324888
H105	0.3155467105	22.1903686508	11.3290870506
H106	0.3513898770	21.7523206672	14.7419363768
H107	-0.4051845731	22.5392301197	13.3431304053

H108	-0.4129706606	19.5414412111	13.9249558334
H109	-1.7689201491	20.6461256958	14.2626731889
H110	-4.1875885313	17.1012252668	6.4017776543
H111	-5.6330533115	18.1041726173	6.6888076539
H112	0.3965330657	20.2129291264	6.9792191502
H113	3.1090696165	17.3119230651	5.7984691579
H114	2.1426080761	21.9010312431	7.1993142324
H115	4.9911631806	18.8403268235	5.9769947418
H116	-1.1622999586	18.0676189859	8.5311333638
H117	2.3465730412	15.8131534019	7.5022611178
H118	-1.1228588401	17.0826370369	10.7886932521
H119	2.4245181220	14.8821905295	9.7692137646
H120	3.7174898754	23.0583877565	7.8884323479
H121	6.4842965825	20.2738786860	5.9888213780
H122	5.6562096190	24.3638317681	8.5557323871
H123	8.2941975756	21.7182202301	6.7402531612
H124	0.4812504325	17.8369590261	12.6703418676
H125	3.2251697976	14.7366800743	12.6027691224
H126	2.1431403152	19.4517315211	13.4196043462
H127	5.0227206435	16.1716389445	13.4044368129
H128	9.0880719430	24.9590036365	10.7065089330
H129	7.2487712092	21.3013235716	9.4048165384
H130	9.0369184996	24.1463055262	13.0307118567
H131	7.2101114787	20.4938131261	11.7009109451
H132	3.6384480536	20.7703877369	13.6190174760
H133	6.4812221754	17.4928836401	14.0855110367
H134	5.5197648686	22.2929599550	13.9303719670

H135	8.2274493150	19.1686749320	14.3247537782
H136	5.1314162163	13.1264045943	10.9086385078
H137	5.2672147849	15.4312878895	6.7280186885
H138	3.1841591530	11.6097416389	10.7404582324
H139	3.9982557929	15.2304060204	4.6041489481
H140	1.8151775975	11.5351635293	8.6814998108
H141	2.0867892723	13.6909792768	4.4161769848
H142	-2.2869168274	18.3422771117	13.8060028990
H143	-3.7596568117	16.5430770951	12.9739633312
H144	-1.5542943429	21.1782157407	10.0142701470
H145	-4.5151747162	16.5109688154	10.6177382490
H146	-2.3347399357	21.1512144407	7.6663961652
H147	-3.7981382988	19.3533309995	6.8382906369
C148	-5.9934836193	16.0069357658	6.8226413266
H149	-6.3370084706	16.0201378330	5.7828647852
H150	-6.8656677387	16.1005177014	7.4774769628
C151	-6.0011920572	13.6694063270	6.6670006204
H152	-7.0587266745	13.7558750347	6.9412343449
H153	-5.9399176581	13.5754481398	5.5778968259
C154	-4.0384751760	11.4274089905	5.7285342300
H155	-3.9811708718	12.1752921443	4.9344190701
H156	-4.9004371238	10.7780616784	5.5401625783
C157	-2.7831009527	10.5628788573	5.6890667439
H158	-2.8080085967	9.9699036712	4.7681972703
H159	-2.7762081937	9.8826489872	6.5459040387
C160	-5.4654050327	12.4217065724	7.3660958510
H161	-6.1645181175	11.5994071527	7.1779324196

H162	-5.4390453118	12.6228657411	8.4365136838
------	---------------	---------------	--------------

1⁺ CBPQT circling glycol chain

-3759.480590	-3759.380247	-3760.419180	-3760.519522
--------------	--------------	--------------	--------------

N1	1.7031512541	18.7236090562	6.4272612881
C2	0.6394053876	17.6940585087	6.4714423128
C3	1.4399592690	20.0049640992	6.7978928881
C4	2.9903957442	18.3602734269	6.1827418459
C5	0.5881583066	17.0511173261	7.8505509981
C6	2.4311618150	20.9281802921	6.9581536548
C7	4.0273308699	19.2341478144	6.3162282712
C8	-0.3677598109	17.4343757007	8.7856437022
C9	1.5477484576	16.0993093430	8.2020418262
C10	3.8061106680	20.5804999494	6.7502858634
C11	-0.3551199093	16.8766976413	10.0654971921
C12	1.5713342424	15.5626349993	9.4821155455
C13	4.8778985603	21.4851456854	6.9969270671
C14	0.6189990764	15.9491320658	10.4268424835
C15	4.6865239611	22.7444381632	7.6576563061
C16	6.2384933986	21.1818602297	6.6528141039
C17	0.7021294088	15.4187508435	11.8549191937
C18	5.7512781062	23.5077869449	8.0264494454
C19	7.2603804928	21.9960318981	7.0393831118
N20	1.7029697113	16.1520744969	12.6337631551
N21	7.0374660457	23.1377509211	7.7515259485
C22	1.4816475667	17.5011968584	12.8655646053
C23	3.0027134589	15.7008724262	12.7477744363

C24	8.1338075270	23.7632765528	8.5046107292
C25	2.4528588046	18.3684393428	13.1948655789
C26	4.0289833262	16.4992659313	13.1008306161
C27	8.1681680135	23.1928851455	9.9263971151
C28	3.8592073031	17.9472249577	13.3060835702
C29	8.8226362646	23.8790648503	10.9546251613
C30	7.5253014673	21.9933680745	10.2249600946
C31	4.8805911397	18.8142625293	13.5567762661
C32	8.8149391014	23.3760421705	12.2555269085
C33	7.5196738062	21.4919261254	11.5230684425
C34	4.6857419287	20.2680037544	13.7165168094
C35	6.2989747092	18.4213990937	13.6600469592
C36	8.1558722282	22.1787136470	12.5540966033
C37	5.7063520553	21.0944905096	13.9963874992
C38	7.2713182918	19.3153069054	13.9275764880
C39	8.0876146739	21.6432593007	13.9889277580
N40	7.0228188500	20.6610511072	14.1566117577
O41	5.8275051268	14.8997616837	9.0528920750
C42	4.8003659413	14.0101999446	9.0432967001
C43	6.1348239571	15.5827402873	10.2698031737
C44	4.0789016351	13.9174034614	7.8090334877
C45	4.4793912428	13.2011174213	10.1053083704
C46	6.1735906223	17.0779588151	9.9941354527
C47	4.4351236331	14.7265778699	6.6894736948
C48	3.0064703052	13.0044784320	7.7203706879
C49	3.3932451068	12.2916196652	9.9948646295
O50	4.8636578632	17.4793219424	9.6687403216

C51	3.7463690177	14.5851981033	5.5164977983
C52	2.2894522309	12.9060586395	6.4765816900
C53	2.6658487681	12.1931988684	8.8387158126
C54	4.5729966628	18.8242497211	10.0006731127
C55	2.6627863282	13.6694307500	5.3978975455
O56	1.2746297197	12.0096090043	6.4674840717
C57	3.0563590961	18.9833816223	9.9869155924
C58	0.7161861804	11.6568388071	5.2059066377
O59	2.7663983500	20.1928062013	10.6616879270
C60	-0.3932948417	10.6331233094	5.4152929973
C61	1.3911093354	20.5010650634	10.6891358221
O62	-1.5847789886	11.3205973641	5.7407491761
C63	1.1949204883	21.7544737615	11.5386063220
O64	1.2673101509	21.4846025921	12.9367775635
C65	0.0767084745	21.6742407919	13.6783030367
O66	-4.1031869679	12.0158542636	6.9991488571
C67	-0.8762238204	20.4869046407	13.5947020152
O68	-1.3783430231	20.4189603880	12.2655949717
C69	-2.1910779565	19.3838318931	11.9235832695
O70	-5.2559556164	14.8040837406	7.1162487302
C71	-2.5806079421	18.3832097367	12.7788000246
C72	-2.6382076660	19.3978912156	10.5579885513
C73	-3.4221002568	17.3383250933	12.3012873274
C74	-3.4734206252	18.3530009738	10.1117444187
C75	-2.2471183351	20.4370815860	9.6645973772
C76	-5.0655938715	17.2042126300	7.0175501842
C77	-3.8577519018	17.3115165832	11.0053340149

C78	-3.9104540373	18.3554504773	8.7412239522
C79	-2.6814456295	20.4076366521	8.3681931888
O80	-4.7186193270	17.3278782236	8.3917340400
C81	-3.5139978710	19.3587818944	7.8890287564
H82	-0.3015252110	18.1817845110	6.2238314435
H83	0.8668527245	16.9591876687	5.7009784506
H84	-0.2659588256	15.5217694213	12.3474376289
H85	0.9800471201	14.3650265478	11.8572692130
H86	9.0629973386	23.5603422090	7.9739568522
H87	7.9714027020	24.8400289749	8.5270740989
H88	7.9160112316	22.4744162787	14.6752229667
H89	9.0331408962	21.1728774738	14.2634313923
H90	5.3462814261	15.4099846448	10.9989187843
H91	7.0933393404	15.2258508671	10.6485702568
H92	6.8729226226	17.3050549772	9.1823642422
H93	6.5177208171	17.5791616048	10.9056743499
H94	4.9135320876	19.0506485467	11.0148004670
H95	5.0441158093	19.5143049516	9.2912336685
H96	2.6157317192	18.1311074582	10.5064800864
H97	2.6770539559	19.0085535749	8.9606224621
H98	0.2828765334	12.5329930155	4.7209112895
H99	1.5030617584	11.2355096729	4.5760389482
H100	-0.5237450208	10.0793433897	4.4800760702
H101	-0.1095775672	9.9295695297	6.2033986308
H102	1.0326097593	20.7010787816	9.6725584633
H103	0.8099868459	19.6728771818	11.1016224646
H104	1.9956906087	22.4530979832	11.2933058479

H105	0.2351420385	22.2135890230	11.3000032442
H106	0.3705846650	21.7918313505	14.7210314231
H107	-0.4409717361	22.5813789285	13.3548555339
H108	-0.3373076781	19.5710069041	13.8427594880
H109	-1.7004820923	20.6263176814	14.2985830274
H110	-4.1599730335	17.0994506141	6.4194234679
H111	-5.6190132446	18.0902153304	6.6957446193
H112	0.3983269582	20.2428659338	6.9631686494
H113	3.1440344316	17.3317702748	5.8908296519
H114	2.1387102076	21.9287050978	7.2392558332
H115	5.0204389335	18.8581569278	6.1219318258
H116	-1.1293728070	18.1609688450	8.5254480726
H117	2.2868881784	15.7753601802	7.4792345227
H118	-1.1165655427	17.1683871580	10.7795593178
H119	2.3376290773	14.8437922305	9.7468556125
H120	3.7052641509	23.0997937599	7.9307837757
H121	6.4953505937	20.3027940274	6.0806195053
H122	5.6341197162	24.4274549958	8.5837440610
H123	8.2946132383	21.7664358937	6.8200246223
H124	0.4502363547	17.8101596723	12.7534759700
H125	3.1388976209	14.6410486900	12.5718042071
H126	2.1728851435	19.4032319646	13.3389762406
H127	4.9971837331	16.0364008212	13.2339427211
H128	9.3206559493	24.8201769987	10.7462109352
H129	6.9967899656	21.4418672421	9.4568619284
H130	9.3070772055	23.9332129503	13.0464166800
H131	6.9870180483	20.5722250842	11.7294704276

H132	3.7072949432	20.7068491575	13.5790985598
H133	6.5969170447	17.3886203203	13.5363210210
H134	5.5652616736	22.1628628297	14.1037208520
H135	8.3120082162	19.0221015342	13.9953233901
H136	5.0585080353	13.2397826760	11.0197624810
H137	5.2460916878	15.4339913287	6.7939660602
H138	3.1505881387	11.6636326601	10.8429965118
H139	4.0213484117	15.1716941211	4.6476871512
H140	1.8380775239	11.5035947133	8.7539502823
H141	2.1465010581	13.5886124406	4.4519877969
H142	-2.2609235423	18.3740504930	13.8122138224
H143	-3.7112830255	16.5531125404	12.9881945908
H144	-1.6209119001	21.2384193080	10.0295763401
H145	-4.4831923587	16.5108948188	10.6371709339
H146	-2.4012189758	21.1977535641	7.6824590083
H147	-3.8316946418	19.3719530631	6.8562291946
C148	-5.9615872096	15.9920979452	6.8279107485
H149	-6.2919082823	16.0017980613	5.7837886157
H150	-6.8428938126	16.0803971874	7.4712475721
C151	-5.9461983459	13.6548677920	6.6593051123
H152	-7.0098204713	13.7310646599	6.9117672353
H153	-5.8605990942	13.5696877229	5.5710150552
C154	-3.9844671871	11.3893266794	5.7370205748
H155	-3.9090197225	12.1264838793	4.9346085971
H156	-4.8538345581	10.7504231615	5.5485399132
C157	-2.7416125425	10.5055350141	5.7200957611
H158	-2.7621304451	9.9068123430	4.8030617426

H159	-2.7556452029	9.8310078868	6.5812402072
C160	-5.4152999566	12.4051772649	7.3592988239
H161	-6.1146797383	11.5847827627	7.1646086391
H162	-5.3950821383	12.6031671293	8.4303061207

1⁰ CBPQT circling glycol chain

-3759.603488 -3759.537672 -3760.586654 -3760.652470

N1	1.4748766132	18.6740910583	6.4017412228
C2	0.4502075558	17.6354571700	6.5425373519
C3	1.2706265324	19.9193696944	6.9695569238
C4	2.7865359748	18.2978792966	6.1775021351
C5	0.4688465141	17.0154209205	7.9332926483
C6	2.2693614235	20.7842025015	7.2279476190
C7	3.8376680350	19.1049289882	6.4010552823
C8	-0.4721868561	17.3826506421	8.8879444540
C9	1.4831458909	16.1213638567	8.2870671902
C10	3.6790132984	20.4587533973	6.9536556043
C11	-0.3990701700	16.8704973037	10.1840630232
C12	1.5657189027	15.6232620986	9.5797857937
C13	4.7228464644	21.2998637110	7.1997034080
C14	0.6231793892	15.9954510407	10.5423667770
C15	4.5873534852	22.6185252756	7.8438176039
C16	6.1245686051	20.9789367320	6.8709816219
C17	0.7698209192	15.5061004808	11.9797111590
C18	5.6504088267	23.3976447310	8.1042466957
C19	7.1380458471	21.8154438129	7.1526512815
N20	1.8185169035	16.2369175021	12.6958332108

N21	6.9555765909	23.0552338119	7.7538552757
C22	1.6189332666	17.5808658799	12.9678888299
C23	3.1201644748	15.7790506802	12.7104654275
C24	8.0550232652	23.6458034473	8.5046388303
C25	2.6094641843	18.4383971715	13.2741699020
C26	4.1680575863	16.5613322452	13.0315267317
C27	8.1687702447	23.0747968430	9.9219194952
C28	4.0144369633	17.9951597396	13.3279270737
C29	8.9900181914	23.6862869270	10.8766655181
C30	7.4370173491	21.9489740258	10.2914756477
C31	5.0615195189	18.8221480278	13.6097557545
C32	9.0610687889	23.1859167224	12.1746223501
C33	7.5118302388	21.4457351874	11.5887523396
C34	4.9106883091	20.2595908559	13.8949790043
C35	6.4721457362	18.3891158693	13.6339070179
C36	8.3148014305	22.0612793387	12.5455512700
C37	5.9609248699	21.0436016931	14.1824926802
C38	7.4766172834	19.2392850869	13.9124096851
C39	8.3410132617	21.5386802541	13.9849642921
N40	7.2760569766	20.5759702032	14.2394668406
O41	5.9827366492	14.9481843997	8.9735688940
C42	4.9153393355	14.1072556226	9.0095865533
C43	6.3654833978	15.6635917558	10.1500724021
C44	4.1438334057	14.0490116900	7.8037144552
C45	4.6206214850	13.2875556943	10.0702966448
C46	6.1961058354	17.1553175194	9.9048677753
C47	4.4632926105	14.8790847617	6.6893414530

C48	3.0708329726	13.1344993725	7.7294517608
C49	3.5217093056	12.3918801857	9.9829620467
O50	4.8220719677	17.4066320867	9.7761747173
C51	3.7482504675	14.7485146496	5.5314537014
C52	2.3271734429	13.0452360370	6.5008674096
C53	2.7624875342	12.3085083349	8.8462028070
C54	4.4819824017	18.7636342368	10.0032447410
C55	2.6718634199	13.8232766574	5.4238888512
O56	1.3195986307	12.1382660568	6.4968849582
C57	2.9620467665	18.8606341416	10.0471849475
C58	0.7653516220	11.7845558442	5.2340828062
O59	2.6568238967	20.1074474492	10.6501042841
C60	-0.3300737949	10.7437105706	5.4334977860
C61	1.2759447390	20.3809715291	10.7068854401
O62	-1.5421821832	11.4079403366	5.7366184163
C63	1.0886814986	21.7255168672	11.4071429335
O64	1.1457971742	21.6189044555	12.8292950302
C65	-0.0753965666	21.8225139082	13.5120148761
O66	-4.0917672542	11.9972948185	6.9951368319
C67	-1.0162371891	20.6238967369	13.4459531684
O68	-1.5143543966	20.5273696952	12.1173256740
C69	-2.3108551982	19.4764750765	11.7901066988
O70	-5.2576902689	14.7541308436	7.0329119161
C71	-2.7179190398	18.5030640120	12.6672438241
C72	-2.7234795422	19.4456813613	10.4147858598
C73	-3.5452670091	17.4414663350	12.2036318416
C74	-3.5467913206	18.3843226123	9.9822770956

C75	-2.3133221670	20.4576936118	9.4995095608
C76	-5.0568700437	17.1489559423	6.8814163117
C77	-3.9495486286	17.3714397721	10.8995823187
C78	-3.9540307033	18.3469001658	8.6031701509
C79	-2.7151581985	20.3865582917	8.1947034578
O80	-4.7580605651	17.3110395995	8.2628582849
C81	-3.5361741809	19.3225203474	7.7297020469
H82	-0.5220473033	18.0867458703	6.3434717913
H83	0.6417785893	16.8762816561	5.7836108951
H84	-0.1710529048	15.6356678745	12.5176410640
H85	1.0328367839	14.4482019643	11.9992791555
H86	8.9801586658	23.4661563575	7.9540001818
H87	7.9019182026	24.7249345588	8.5575969534
H88	8.2296412160	22.3769642753	14.6750501333
H89	9.2965399260	21.0562853256	14.1965726894
H90	5.7226912385	15.3904651058	10.9837501412
H91	7.4030418073	15.4182335077	10.3754330440
H92	6.7426842973	17.4606217542	9.0051220790
H93	6.6114882797	17.6921895150	10.7664497898
H94	4.8625829648	19.0874788956	10.9764988597
H95	4.8840741598	19.4048326706	9.2124818860
H96	2.5788314914	18.0347405790	10.6487928658
H97	2.5408957922	18.7999147805	9.0420494861
H98	0.3218520249	12.6556866505	4.7511702111
H99	1.5586931106	11.3786097808	4.6023051963
H100	-0.4360280456	10.1834325484	4.4990415554
H101	-0.0452602008	10.0484701399	6.2287352790

H102	0.8646028021	20.4399064241	9.6949559502
H103	0.7383078231	19.5972216138	11.2478378055
H104	1.9031471614	22.3773823803	11.0903006971
H105	0.1391320416	22.1728026885	11.1121597368
H106	0.1742235640	21.9923632317	14.5592245885
H107	-0.5933781928	22.7062059664	13.1272132761
H108	-0.4688749062	19.7177376971	13.7134535658
H109	-1.8450105683	20.7692674196	14.1438333361
H110	-4.1290062411	17.0204160544	6.3240908920
H111	-5.5907591633	18.0276808494	6.5106872285
H112	0.2377201109	20.1561818534	7.1920997169
H113	2.9154836258	17.2930215951	5.8008801669
H114	2.0020255093	21.7387827467	7.6583757255
H115	4.8192592526	18.7065644521	6.1897776628
H116	-1.2675555339	18.0704250556	8.6269891852
H117	2.2233048344	15.8201862722	7.5558323241
H118	-1.1499717988	17.1594520306	10.9100571674
H119	2.3758796327	14.9520560858	9.8404430001
H120	3.6170220806	22.9853557139	8.1448688512
H121	6.3726497739	20.0536422722	6.3714133572
H122	5.5495817827	24.3528596043	8.6045816451
H123	8.1657158113	21.5688230615	6.9151768628
H124	0.5871169116	17.8981749523	12.8982770546
H125	3.2438305871	14.7312181393	12.4685215280
H126	2.3413678365	19.4738151544	13.4295880683
H127	5.1424586539	16.0947482548	13.0660225818
H128	9.5629231336	24.5686221531	10.6089803497

H129	6.7811913555	21.4631137535	9.5805741806
H130	9.6864122724	23.6839183998	12.9087813440
H131	6.9142451242	20.5819032725	11.8503152545
H132	3.9349212963	20.7224562716	13.8520086809
H133	6.7378637843	17.3609277053	13.4330075222
H134	5.8475636014	22.1026213983	14.3773030222
H135	8.5113288645	18.9197059988	13.9129072586
H136	5.2358859612	13.2968606556	10.9612604333
H137	5.2676539261	15.5946428166	6.7855273013
H138	3.3004525977	11.7553465738	10.8305968350
H139	3.9952851890	15.3527686775	4.6663377230
H140	1.9313132678	11.6211165498	8.7756236202
H141	2.1361051839	13.7500763971	4.4879205288
H142	-2.4206930578	18.5273650600	13.7069253862
H143	-3.8476735281	16.6761653444	12.9073593822
H144	-1.6962252431	21.2707214548	9.8534444352
H145	-4.5633243091	16.5572118150	10.5417953725
H146	-2.4169868933	21.1539327674	7.4907746369
H147	-3.8266326578	19.3022417605	6.6887869054
C148	-5.9519202781	15.9359204797	6.6957977666
H149	-6.2538701092	15.9193344338	5.6433934425
H150	-6.8503171625	16.0433033233	7.3120827991
C151	-5.9531849241	13.5975976159	6.6077933666
H152	-7.0152156045	13.6807145125	6.8648119143
H153	-5.8751690781	13.4865789470	5.5220989441
C154	-3.9424308201	11.4025734979	5.7217302264
H155	-3.8802992841	12.1582170221	4.9364415213

H156	-4.7917041856	10.7441159353	5.5109329403
C157	-2.6733497934	10.5578694646	5.7007783174
H158	-2.6688370784	9.9700874182	4.7766178360
H159	-2.6711379166	9.8725243685	6.5533056781
C160	-5.4145023125	12.3676422533	7.3329088239
H161	-6.0978113082	11.5331145847	7.1460624587
H162	-5.4104732632	12.5857911284	8.3987848879

2⁴⁺ CBPQT circling HQ

-3451.877057 -3451.211417 -3452.161349 -3452.826989

O1	10.2164558295000	5.7107605994000	22.0295659920000
C2	11.4910132629000	5.2263470445000	22.4180424917000
C3	9.9964332581000	5.9430998576000	20.7044303025000
C4	11.5103473349000	5.1185199769000	23.9317042645000
C5	10.9007706158000	5.6168813503000	19.6859736033000
C6	8.7728582584000	6.5221192035000	20.3723869028000
O7	10.6537745121000	4.0621270083000	24.3250924894000
C8	10.5627869175000	5.8537028783000	18.3564580175000
C9	8.4263556823000	6.7429674897000	19.0406009238000
C10	10.6790078872000	3.8246697575000	25.7239033736000
C11	9.3234841621000	6.3990476525000	18.0226363520000
C12	10.0791555420000	2.4589543880000	25.9956420047000
O13	9.0662580193000	6.5308422413000	16.6902482560000
O14	8.7050620163000	2.4470833651000	25.6374177314000
C15	7.8114994012000	7.0568041183000	16.2932331376000
C16	8.1215411204000	1.1897185583000	25.9512651494000
C17	7.7805839622000	7.0981217077000	14.7756197740000

C18	6.6290303665000	1.2067763727000	25.6774392120000
O19	7.7707405961000	5.7759289370000	14.2671126686000
O20	6.4000894660000	1.2881231876000	24.2796325634000
C21	7.6070994369000	5.7466338193000	12.8563297113000
C22	5.1804537191000	0.6767364068000	23.8986018125000
C23	7.5106880511000	4.3022290252000	12.4002983570000
C24	5.0003928639000	0.8354446402000	22.4004174367000
O25	8.7616123036000	3.6645451683000	12.6092059635000
O26	6.1038641749000	0.2071221466000	21.7733501643000
C27	8.8875049971000	2.4231296410000	11.9281568391000
C28	6.2429632313000	0.3512786815000	20.4257013077000
C29	7.7540872355000	1.4532387130000	12.2584326561000
C30	5.2933066233000	0.9295543306000	19.5938570267000
C31	7.4430612457000	-0.1301399500000	19.8804354816000
O32	7.5570543560000	1.4520933695000	13.6603725784000
C33	5.5413206172000	1.0444763684000	18.2177937749000
C34	7.6795906805000	-0.0308113213000	18.5224034578000
C35	6.4792139799000	0.6157748578000	14.0387260373000
C36	6.7289507904000	0.5640012237000	17.6796444133000
C37	6.0252893996000	0.9686771570000	15.4427393545000
O38	7.0591886084000	0.6318631603000	16.3568213096000
H39	11.6791538362000	4.2416302302000	21.9845888187000
H40	12.2723622040000	5.9199979979000	22.0971834526000
H41	12.5350866312000	4.9115608820000	24.2535476086000
H42	11.1873950627000	6.0666838772000	24.3718622455000
H43	11.8600716665000	5.1700258707000	19.9123918363000
H44	8.0879751828000	6.7764165589000	21.1740961842000

H45	11.2470597445000	5.5961457915000	17.5549348542000
H46	7.4589107117000	7.1707839656000	18.8122321942000
H47	11.7102064658000	3.8231332535000	26.0887197887000
H48	10.1191839919000	4.5997027403000	26.2564077746000
H49	10.6223497691000	1.7052368512000	25.4188595869000
H50	10.1877698000000	2.2364044078000	27.0616026741000
H51	6.9968203620000	6.4274809953000	16.6596711145000
H52	7.6832780081000	8.0719832263000	16.6782942447000
H53	8.5867289564000	0.4022483256000	25.3529784569000
H54	8.2753508512000	0.9689011121000	27.0120487921000
H55	6.8761702429000	7.6284515264000	14.4636852622000
H56	8.6536081203000	7.6434644658000	14.4063391543000
H57	6.1542927971000	2.0474946172000	26.1921927292000
H58	6.2135389893000	0.2762970916000	26.0742165768000
H59	6.6853159779000	6.2656269364000	12.5774332658000
H60	8.4533231416000	6.2364202900000	12.3648344405000
H61	5.2010838968000	-0.3869214701000	24.1514705163000
H62	4.3322238187000	1.1459475843000	24.4063685626000
H63	6.7291524497000	3.7927412322000	12.9689484927000
H64	7.2544741150000	4.2917884853000	11.3364830381000
H65	4.0610282151000	0.3662920575000	22.0979178624000
H66	4.9718688947000	1.8950532679000	22.1342890571000
H67	8.9080346031000	2.5848705968000	10.8461759196000
H68	9.8406725300000	1.9955656523000	12.2345050921000
H69	8.0273686477000	0.4572276537000	11.8957198644000
H70	6.8302177572000	1.7566968936000	11.7564770492000
H71	4.3544762659000	1.2993745710000	19.9848475689000

H72	8.1698053417000	-0.5831197046000	20.5433991715000
H73	4.7890041293000	1.5062099393000	17.5925322778000
H74	8.5955857698000	-0.4103977563000	18.0861240655000
H75	5.6271746739000	0.7706100114000	13.3691301120000
H76	6.7744821432000	-0.4364522966000	13.9939959921000
H77	5.1245833945000	0.3932969424000	15.6693865302000
H78	5.8015964143000	2.0365494599000	15.4992981041000
C79	10.4465772222000	9.6893645414000	20.4088772930000
C80	9.0707230979000	9.9172013455000	20.2921858378000
C81	11.0146601930000	9.7022961502000	21.6845917917000
C82	11.2724636568000	9.3925250201000	19.1975909677000
C83	8.3060641952000	10.0587637968000	21.4325289289000
C84	10.1968037970000	9.8461294625000	22.7919151645000
C85	12.4294362238000	8.6135443449000	19.3012381602000
C86	10.8910436017000	9.8489330956000	17.9330677922000
N87	8.8698342844000	9.9847181401000	22.6501461678000
C88	13.1402540894000	8.2969557553000	18.1586091588000
C89	11.6361513933000	9.4890495935000	16.8244475946000
N90	12.7274510919000	8.7181138103000	16.9519582207000
C91	7.5067960776000	8.4350082173000	23.9189018633000
C92	8.3921407460000	7.4489592873000	24.3604952011000
C93	6.2452531293000	8.0685314007000	23.4481861482000
C94	12.8929367263000	6.8536873031000	15.3824914286000
C95	8.0431265594000	6.1055646459000	24.2784342363000
C96	5.8837258167000	6.7209372236000	23.3911313335000
C97	13.5362403404000	5.6991680342000	15.8362453171000
C98	11.6921246334000	6.7452169343000	14.6819715194000

C99	6.7908357948000	5.7354384629000	23.7834856967000
C100	12.9518253347000	4.4490231146000	15.6360890054000
C101	11.1006412319000	5.4987976888000	14.4929302524000
C102	6.4707421267000	4.2549836202000	23.6402623384000
C103	11.7169127369000	4.3507247487000	14.9905433213000
N104	7.0095174059000	3.7754453262000	22.3316319662000
C105	10.9759212011000	3.0238409720000	14.9016666160000
C106	8.1941066724000	3.1519293032000	22.2918480725000
C107	6.3365688596000	4.0623892418000	21.2027035022000
N108	10.1582870575000	2.8765686006000	16.1413626001000
C109	8.7759723440000	2.8409857975000	21.0707567643000
C110	6.8656643886000	3.7637780762000	19.9657718827000
C111	8.9294723165000	3.4087146515000	16.1725069897000
C112	10.7091252354000	2.3273400620000	17.2384455475000
C113	8.1321232550000	3.1718123316000	19.8762888512000
C114	8.2291469612000	3.4669185176000	17.3668400865000
C115	10.0524203538000	2.3589389952000	18.4487617926000
C116	8.7989191325000	2.9777249896000	18.5440099369000
H117	8.5647002734000	9.9445316398000	19.3373057746000
H118	12.0796110055000	9.6064791829000	21.8464342446000
H119	7.2347479478000	10.2049355230000	21.3967802034000
H120	10.5869702237000	9.8452074131000	23.8002503116000
H121	12.7914089132000	8.2306205273000	20.2448729735000
H122	10.0387839683000	10.4976513353000	17.7836530035000
H123	14.0407918286000	7.6986429558000	18.1857338558000
H124	11.3793486270000	9.8188851386000	15.8274823361000
H125	9.3596836451000	7.7285045948000	24.7614163742000

H126	5.5390916560000	8.8258562775000	23.1274091176000
H127	8.7525080944000	5.3365692287000	24.5632207578000
H128	4.8955972820000	6.4488985098000	23.0373621701000
H129	14.4902356816000	5.7691144751000	16.3463535622000
H130	11.2102363835000	7.6331787935000	14.2894580869000
H131	13.4589757111000	3.5592712554000	15.9913733673000
H132	10.1458822308000	5.4151905326000	13.9866086722000
H133	6.9594471156000	3.6624872087000	24.4084375253000
H134	5.4001249209000	4.0624939417000	23.6452305606000
H135	10.2743287004000	3.0297713119000	14.0731259988000
H136	11.6447366682000	2.1685339482000	14.8420998015000
H137	8.6687187125000	2.9444888034000	23.2440487276000
H138	5.3771877597000	4.5487109973000	21.3145408710000
H139	9.7428244839000	2.3605866393000	21.0964228123000
H140	6.2733229264000	4.0179661150000	19.1001970753000
H141	8.5452108780000	3.8199477643000	15.2456569314000
H142	11.6863042822000	1.8778702658000	17.1251513300000
H143	7.2540515378000	3.9278033230000	17.3414760694000
H144	10.5480403061000	1.9045671708000	19.2937360667000
C145	7.9764269968000	9.8827190165000	23.8476126855000
H146	8.5630845338000	10.1737813947000	24.7153013072000
H147	7.1545949249000	10.5798166208000	23.7064550478000
C148	13.4415853875000	8.2303535284000	15.7272822141000
H149	13.2566719506000	8.9566797202000	14.9397080148000
H150	14.5030475063000	8.2071941661000	15.9608739574000

2³⁺ CBPQT circling BQ

-3452.029752 -3451.641784 -3452.594904 -3452.982873

O1	6.4680313104	6.6758684336	16.4019533080
C2	7.8184821200	6.8344131817	16.2715916426
C3	5.9371256175	5.3661753678	16.3052979311
C4	8.7380968540	5.7799500752	16.2373272887
C5	8.2756742995	8.1478497088	16.2087756962
H6	6.3269277658	4.7275140760	17.1017353620
H7	6.1866893957	4.9268902612	15.3360967942
C8	4.4277262693	5.4603932412	16.4466665762
C9	10.0994377864	6.0548167927	16.1474375394
H10	8.4105372791	4.7494048248	16.2703270710
H11	7.5458975788	8.9483894447	16.2260920292
C12	9.6376362551	8.4232215623	16.1226809472
O13	4.1195510753	5.8081112857	17.7858114607
H14	4.0393949720	6.2090734265	15.7510919417
H15	3.9908450621	4.4878338547	16.2027891530
C16	10.5564974983	7.3693734017	16.0918555669
H17	10.8306403398	5.2546459054	16.1110571974
H18	9.9647145643	9.4537690727	16.0743527995
C19	2.7265913356	5.8511755397	18.0473806980
O20	11.9118103274	7.5325103134	16.0449262582
H21	2.2337092416	4.9666057291	17.6336556358
H22	2.2770637400	6.7417432070	17.5985156225
C23	2.5144340973	5.8519554247	19.5508022667
C24	12.4165237331	8.8245303870	15.7625784130
O25	3.1505468141	6.9800203015	20.1294809784
H26	1.4386678003	5.8793499037	19.7509689598

H27	2.9289270349	4.9347111698	19.9757024082
C28	13.9106593897	8.7048014244	15.5252459677
H29	12.2331734297	9.5067141206	16.5966110068
H30	11.9462213843	9.2261412624	14.8614606227
C31	2.9161693386	7.0386268336	21.5294139242
O32	14.5606311242	8.3697202735	16.7385170298
H33	14.0967126102	7.9378533302	14.7682255754
H34	14.2775246348	9.6669293607	15.1546002082
H35	3.1905096402	6.0852834233	21.9915277368
H36	1.8551217936	7.2255457285	21.7219365976
C37	3.7440734731	8.1662142933	22.1320827510
C38	15.9723050292	8.4511164236	16.6174132491
O39	5.1354504277	7.8777689780	22.0784369254
H40	3.5687509007	9.0851778856	21.5742071598
H41	3.4260668290	8.3313151561	23.1648752666
C42	16.6122112866	8.0269525515	17.9281351212
H43	16.2683191208	9.4796457628	16.3885891055
H44	16.3230240360	7.7941998342	15.8149115703
C45	5.5902005142	7.2214184578	23.2516436982
O46	16.3856584858	6.6402237024	18.1072514657
H47	17.6856692836	8.2344909169	17.8731973204
H48	16.1735900449	8.5955511760	18.7521662098
H49	4.9417964000	6.3780810486	23.5034982498
H50	5.5964480345	7.9212699819	24.0923428015
C51	6.9908086608	6.6770286030	23.0401067709
C52	17.2194561548	6.0231851888	19.0725713231
O53	7.8669293071	7.7734688669	22.8319004889

H54	7.2782288809	6.1232824023	23.9370123053
H55	7.0139587348	6.0118133558	22.1749007518
C56	17.1239528080	6.6974573179	20.4398996007
H57	18.2636446955	6.0420921047	18.7444970222
H58	16.8907584096	4.9871063910	19.1409066889
C59	9.2049889439	7.5199019586	22.7510965662
O60	15.7554911577	6.8746947043	20.7565485515
H61	17.6244116641	6.0704572844	21.1843009960
H62	17.6264895008	7.6694095279	20.4195215311
C63	9.7862496807	6.2569429943	22.8719670333
C64	10.0206548739	8.6306341391	22.5256009260
C65	15.5771679748	7.6173918451	21.9482141730
H66	9.1887797689	5.3783292226	23.0757952453
C67	11.1653982366	6.1149153459	22.7137365959
C68	11.3906194574	8.4877463472	22.3513958186
H69	9.5598276031	9.6097188812	22.4773894556
C70	14.1411853733	8.0971667718	22.0298245835
H71	16.2221723359	8.5017150111	21.9419148822
H72	15.8204997343	7.0088656985	22.8240695071
H73	11.6273923355	5.1392049097	22.8010308055
C74	11.9683720149	7.2129404100	22.4200764114
H75	11.9893786800	9.3676876607	22.1606680596
O76	13.2957471679	6.9702379279	22.2079713835
H77	14.0442570338	8.7792824020	22.8777535500
H78	13.8828225250	8.6215675931	21.1063321121
N79	11.6815217401	4.5889475671	12.9001628894
C80	10.3863319064	4.1805510494	13.0116673062

C81	11.9438675252	5.9112523969	12.7082231116
C82	12.7941212564	3.6587704427	13.1860601700
H83	10.2328966089	3.1182277322	13.1419984042
C84	9.3467479956	5.0606149880	12.9619484272
C85	10.9514938533	6.8414249378	12.6623161075
H86	12.9835172640	6.1763911230	12.5782366904
C87	13.1610214031	3.7840336998	14.6595312315
H88	13.6298881182	3.9312603063	12.5446357850
H89	12.4643893262	2.6527718971	12.9358593620
H90	8.3519421249	4.6535051140	13.0599607394
C91	9.5776689065	6.4688469582	12.8239342953
H92	11.2416101295	7.8634490503	12.4731950776
C93	12.5502511195	2.9681180349	15.6161640710
C94	14.0278696891	4.7931273346	15.0755588979
C95	8.5261933210	7.4263142643	12.8527654520
C96	12.7670542946	3.1957003291	16.9735086073
H97	11.9026717826	2.1564983051	15.3039395800
H98	14.5473611003	5.3986558065	14.3413734514
C99	14.2291699163	5.0395287713	16.4323722533
C100	7.1452551854	7.0462462943	12.8682853764
C101	8.7628282597	8.8402666023	12.8742146264
C102	13.5831305161	4.2537722993	17.3846236187
H103	12.2906873788	2.5511777382	17.7038765856
H104	14.8790713191	5.8422610365	16.7581315180
H105	6.8426831373	6.0142775893	12.7791085198
C106	6.1585652904	7.9783280936	12.9632775313
C107	7.7298890109	9.7231497218	12.9816747446

H108	9.7599396465	9.2515712616	12.8331703829
C109	13.6967951224	4.6200270489	18.8570363993
N110	6.4323054683	9.3106853605	13.0404218372
H111	5.1129963988	7.7045241765	12.9641280965
H112	7.8913734041	10.7915055179	13.0262672760
N113	12.4719662099	5.3940904702	19.2188127748
H114	13.7322487556	3.7475675794	19.5038728709
H115	14.5441811174	5.2738221847	19.0512643297
C116	5.3518943658	10.2597667901	13.3844270513
C117	12.4486586095	6.7091087805	18.9570537831
C118	11.3820251147	4.7473218930	19.6633046821
H119	4.4520788524	9.9471645028	12.8575603854
H120	5.6469205566	11.2467674364	13.0350432789
C121	5.1511338913	10.2316727797	14.8949227042
C122	11.2723445934	7.4234631005	19.1068948847
H123	13.3638902190	7.1505942831	18.5790938903
H124	11.4902056302	3.6933211820	19.8787230881
C125	10.1807425221	5.4095613268	19.8172984145
C126	5.8325238856	11.1269736263	15.7235896949
C127	4.3780738584	9.2231408013	15.4684778735
C128	10.1036191619	6.7683970797	19.5018596874
H129	11.2804780968	8.4725435560	18.8491067957
H130	9.3307258851	4.8477123402	20.1778556894
H131	6.4088631284	11.9366594032	15.2905442513
C132	5.7858826533	10.9780028562	17.1090082431
C133	4.3580306276	9.0536641916	16.8495876223
H134	3.8039154485	8.5539914709	14.8383705423

C135	8.7996637569	7.4960751541	19.5365612108
H136	6.3173863529	11.6824333615	17.7385467229
C137	5.0767898745	9.9146878314	17.6740320180
H138	3.8144372054	8.2284851747	17.2912615727
C139	8.7625601148	8.8888421399	19.6791748014
C140	7.5961152369	6.8135285508	19.3769734727
C141	5.1502564605	9.6093237499	19.1622990397
C142	7.5508924227	9.5372688298	19.6170058917
H143	9.6525483593	9.4788044572	19.8416176720
H144	7.5596551643	5.7408465513	19.2494939562
C145	6.4006251036	7.5176950014	19.3169169167
N146	6.4105200111	8.8521130922	19.4125085626
H147	4.3299611947	8.9634285937	19.4671712491
H148	5.1797996052	10.5078867766	19.7745950701
H149	7.4652870149	10.6102799828	19.7169383397
H150	5.4399961667	7.0382845978	19.1584633464

2²⁺ CBPQT circling BQ

-3452.161629 -3451.963664 -3452.922015 -3453.119981

O1	6.5058767812	6.6605603914	16.3598848667
C2	7.8612998784	6.8051223032	16.2533488878
C3	5.9834368849	5.3492113047	16.3798734293
C4	8.7715121687	5.7428024616	16.2451744794
C5	8.3337964622	8.1104288693	16.1613966149
H6	6.3813054818	4.7839885313	17.2263369349
H7	6.2307354534	4.8282549803	15.4502669820
C8	4.4720261348	5.4361012679	16.5170126213

C9	10.1356854058	5.9971373634	16.1390992506
H10	8.4340486615	4.7176242285	16.3168886983
H11	7.6148793586	8.9200648355	16.1782911550
C12	9.6979419212	8.3650559131	16.0573822994
O13	4.1531630916	5.8112271487	17.8448944443
H14	4.0820727393	6.1638409853	15.7996645342
H15	4.0413774612	4.4549155143	16.2944978686
C16	10.6075978609	7.3027295279	16.0407031694
H17	10.8563450957	5.1875829309	16.1337031989
H18	10.0340382277	9.3910745833	15.9918624696
C19	2.7612652870	5.8502858712	18.1012717091
O20	11.9631180059	7.4498727219	15.9347735633
H21	2.2677391942	4.9732120006	17.6710909463
H22	2.3134119733	6.7498864429	17.6680418857
C23	2.5420832033	5.8248054120	19.6040758942
C24	12.4641792897	8.7601603915	15.7834571707
O25	3.1125312493	6.9781744744	20.1970359257
H26	1.4650656601	5.7911310071	19.7999050026
H27	3.0060492754	4.9256526277	20.0189239575
C28	13.9647418273	8.6880316159	15.5586521600
H29	12.2578827163	9.3606489081	16.6731114221
H30	12.0090150572	9.2422878986	14.9133495927
C31	2.8683554136	7.0170754969	21.5938534519
O32	14.6196234872	8.3377176606	16.7632377786
H33	14.1768307035	7.9519365038	14.7778046140
H34	14.3081480485	9.6708361028	15.2190971017
H35	3.1433684817	6.0591269896	22.0463034799

H36	1.8045789206	7.1947661560	21.7837342262
C37	3.6874389442	8.1426085956	22.2149996096
C38	16.0292805596	8.4099166126	16.6447073852
O39	5.0784189190	7.8711559102	22.1636858923
H40	3.5115661020	9.0625929456	21.6587190477
H41	3.3613417840	8.2977615591	23.2476589504
C42	16.6596531463	7.9998278674	17.9653520085
H43	16.3345990711	9.4340537171	16.4051845761
H44	16.3814676765	7.7417162546	15.8518585455
C45	5.5398048255	7.1300641886	23.2788465181
O46	16.4335805053	6.6156290761	18.1590273214
H47	17.7337153573	8.2089638230	17.9192455042
H48	16.2109620285	8.5783858304	18.7769759551
H49	4.8991909677	6.2651843642	23.4700570837
H50	5.5467949966	7.7618957994	24.1723925975
C51	6.9431441848	6.6141849340	23.0121883393
C52	17.2273293950	6.0258883060	19.1731545497
O53	7.8091062045	7.7287407974	22.8937733926
H54	7.2407367720	5.9888852816	23.8577022873
H55	6.9608018233	6.0271063886	22.0927984177
C56	17.0988431256	6.7394925357	20.5183408315
H57	18.2829557213	6.0256640095	18.8808535222
H58	16.8878454336	4.9954062886	19.2651975863
C59	9.1475149642	7.4945501238	22.7552298316
O60	15.7259709703	6.9249724145	20.8028023476
H61	17.5839795438	6.1313313756	21.2889058668
H62	17.6049782466	7.7095557875	20.4842576577

C63	9.7400131723	6.2323301285	22.8030500792
C64	9.9477413208	8.6210906073	22.5629806239
C65	15.5238019385	7.6887373133	21.9766101884
H66	9.1480013052	5.3385390238	22.9473656259
C67	11.1195337358	6.1113963005	22.6437893113
C68	11.3210329607	8.4992727577	22.3925243352
H69	9.4728135140	9.5933605583	22.5289145527
C70	14.0779395791	8.1452227660	22.0448500255
H71	16.1551884130	8.5831868796	21.9574555508
H72	15.7729170040	7.1022857067	22.8665065307
H73	11.5909097267	5.1370319603	22.6659508691
C74	11.9137081936	7.2316384089	22.4243462354
H75	11.9109156862	9.3903965116	22.2260619676
O76	13.2522970192	7.0109055149	22.2464134238
H77	13.9744089282	8.8434196545	22.8799097491
H78	13.8090177662	8.6477382259	21.1125699419
N79	11.6338136848	4.6192038507	12.8965816717
C80	10.3416625432	4.2033481469	13.0183173860
C81	11.8863210172	5.9446425425	12.7136845915
C82	12.7552998302	3.6908464697	13.1597100447
H83	10.1958072661	3.1409923022	13.1581141142
C84	9.2953886831	5.0761263997	12.9691487599
C85	10.8879832876	6.8683159474	12.6700627337
H86	12.9241754920	6.2182098551	12.5894903947
C87	13.1419133932	3.7878019752	14.6291633476
H88	13.5816873466	3.9767814423	12.5109918955
H89	12.4265315775	2.6877218975	12.8963600872

H90	8.3034150207	4.6644086502	13.0775407292
C91	9.5154127803	6.4850057456	12.8195930865
H92	11.1731252121	7.8955065653	12.4986504731
C93	12.5964875927	2.9121705595	15.5710141834
C94	13.9613517679	4.8296187906	15.0643282881
C95	8.4550223283	7.4328694438	12.8247386480
C96	12.8310006379	3.1102802130	16.9312353550
H97	11.9838582586	2.0781375549	15.2465812703
H98	14.4286297278	5.4872665566	14.3402920146
C99	14.1728703084	5.0472257407	16.4233548830
C100	7.0764854172	7.0443227803	12.8262038249
C101	8.6800066284	8.8487632425	12.8334398744
C102	13.5924570607	4.1988142295	17.3656250787
H103	12.4038183875	2.4211264583	17.6514495868
H104	14.7681227323	5.8876637070	16.7606459947
H105	6.7809671363	6.0095021413	12.7452409534
C106	6.0834681748	7.9713246975	12.9054625664
C107	7.6431739182	9.7258415979	12.9333085450
H108	9.6756164952	9.2650971324	12.8031183708
C109	13.6945587832	4.5424753093	18.8462670337
N110	6.3475778710	9.3058471771	12.9824350907
H111	5.0395211951	7.6922884717	12.8968895395
H112	7.7989236996	10.7949033265	12.9821202428
N113	12.5138741547	5.3334964749	19.2292821980
H114	13.7202739768	3.6481871208	19.4671044272
H115	14.5672417770	5.1591689451	19.0463394335
C116	5.2701278749	10.2474677118	13.3529009532

C117	12.5356217977	6.6880498543	19.0905233464
C118	11.3314448724	4.7018714231	19.4816599546
H119	4.3570744279	9.9200882191	12.8579228872
H120	5.5436486322	11.2335235359	12.9826105913
C121	5.1213456438	10.2373156830	14.8695236579
C122	11.3985362668	7.4291531356	19.2133785872
H123	13.4979135933	7.1241312844	18.8540753266
H124	11.3829300982	3.6291558136	19.6081155306
C125	10.1623008033	5.3850262258	19.5836167228
C126	5.7472124604	11.2027998405	15.6606794447
C127	4.4572936504	9.1761955311	15.4878362655
C128	10.1269231182	6.8097397398	19.4357780163
H129	11.4853802578	8.4988088876	19.0888925243
H130	9.2713271361	4.8177134423	19.8084622461
H131	6.2480499182	12.0454260462	15.1961086784
C132	5.7397614711	11.0853088010	17.0515169930
C133	4.4829552217	9.0385983647	16.8715689794
H134	3.9353333196	8.4408032021	14.8864699949
C135	8.9116324705	7.5428851893	19.4809365691
H136	6.2231485450	11.8469196136	17.6538294800
C137	5.1345715114	9.9846762700	17.6625320388
H138	4.0375985959	8.1700023169	17.3429785143
C139	8.8768674759	8.9753221192	19.5027021649
C140	7.6316522796	6.9056875397	19.4929767928
C141	5.2582882309	9.7343694114	19.1608411353
C142	7.6913195290	9.6398188978	19.4723731218
H143	9.7816505198	9.5625579153	19.5565472580

H144	7.5402712412	5.8302657292	19.4849675362
C145	6.4741340318	7.6262753740	19.4525399960
N146	6.4959452606	8.9840689849	19.4278869178
H147	4.4292082103	9.1219396282	19.5098423325
H148	5.2916422440	10.6667583730	19.7227013458
H149	7.6378084829	10.7196210531	19.4886118546
H150	5.4972841602	7.1602065564	19.4222406017

2¹⁺ CBPQT circling BQ

-3452.259894 -3452.163706 -3453.131522 -3453.227710

O1	6.7350690609	6.5210899960	16.3800252879
C2	8.0881749072	6.6917628451	16.2536421013
C3	6.2517943347	5.2076905939	16.5409142332
C4	9.0176791626	5.6486059764	16.2742976951
C5	8.5329788696	8.0000858585	16.0936203891
H6	6.6349304238	4.7610000373	17.4619341868
H7	6.5460539353	4.5860265699	15.6896052063
C8	4.7334288245	5.2634498380	16.6008654497
C9	10.3721152646	5.9195905199	16.1159313872
H10	8.7054693154	4.6238064645	16.4226135624
H11	7.8022728961	8.7983016546	16.1105085729
C12	9.8881246554	8.2720217917	15.9352693090
O13	4.3299108917	5.7511583391	17.8676228950
H14	4.3700663071	5.9120543536	15.7985267132
H15	4.3311478198	4.2569572305	16.4477056248
C16	10.8151171706	7.2258732115	15.9376244875
H17	11.1067563922	5.1254990990	16.1534033043

H18	10.2063696434	9.2993694503	15.8213473194
C19	2.9304378938	5.9380712419	17.9701278405
O20	12.1623204696	7.3893884794	15.7608693608
H21	2.3993113428	5.1375137698	17.4456496490
H22	2.6418382736	6.8973931129	17.5304107643
C23	2.5238656997	5.8829271799	19.4334229093
C24	12.6667242124	8.7030306938	15.7042866993
O25	3.0798802138	6.9768366126	20.1361391741
H26	1.4301476540	5.9099616652	19.4945600176
H27	2.8761227707	4.9404924746	19.8630227080
C28	14.1769951304	8.6346188487	15.5325926634
H29	12.4269773022	9.2496094642	16.6197196740
H30	12.2483365476	9.2388167596	14.8456637641
C31	2.7455965693	6.9403455254	21.5118104328
O32	14.7822314261	8.2232037129	16.7433112795
H33	14.4156059361	7.9360632534	14.7247999594
H34	14.5417335543	9.6291440918	15.2535118412
H35	3.0061276257	5.9645242061	21.9337251402
H36	1.6687800607	7.0939407365	21.6451461797
C37	3.5008564474	8.0495053933	22.2363448484
C38	16.1947550151	8.1964995397	16.6666788537
O39	4.8996129433	7.8343068120	22.2233354469
H40	3.3143216624	8.9945526994	21.7270024278
H41	3.1279499209	8.1282974283	23.2624349109
C42	16.7610710128	7.8838358470	18.0434338443
H43	16.5730861689	9.1739853281	16.3480837813
H44	16.5284932478	7.4392031565	15.9493869751

C45	5.3558774274	6.9941248638	23.2663344000
O46	16.5031034207	6.5278888407	18.3582502975
H47	17.8407751541	8.0697463215	18.0276717598
H48	16.2899793495	8.5427684798	18.7769514913
H49	4.7331484555	6.0999852983	23.3572701023
H50	5.3315530270	7.5318669105	24.2198055678
C51	6.7759101092	6.5403086372	22.9714402758
C52	17.2093397487	6.0539385715	19.4916890062
O53	7.6101804123	7.6830346089	22.9661444769
H54	7.0797953534	5.8453033414	23.7594895839
H55	6.8199390534	6.0465319349	22.0006398432
C56	16.9936084521	6.9069170338	20.7416849589
H57	18.2841680645	6.0138941680	19.2831690412
H58	16.8487372519	5.0431413832	19.6745577181
C59	8.9482505779	7.5072356028	22.7408168113
O60	15.6068040099	7.1027278155	20.9180471493
H61	17.4332101184	6.3845070912	21.5986858592
H62	17.4993943115	7.8728452101	20.6402598287
C63	9.5911685248	6.2685507033	22.7373026145
C64	9.6946015259	8.6654791282	22.5379047495
C65	15.3173802296	7.9679795797	21.9972496507
H66	9.0351872123	5.3485475930	22.8575967309
C67	10.9711478606	6.2089665832	22.5654767533
C68	11.0709416653	8.6047658880	22.3516982441
H69	9.1767980017	9.6146563877	22.5038851631
C70	13.8481928004	8.3529799364	21.9723830488
H71	15.9068629714	8.8874861836	21.9123886519

H72	15.5566032032	7.4876689536	22.9518574661
H73	11.4824544538	5.2557843819	22.5470208179
C74	11.7195210639	7.3672165697	22.3826777789
H75	11.6192654413	9.5202772140	22.1765552879
O76	13.0745515248	7.2063071946	22.2691868054
H77	13.6913013514	9.1260990183	22.7301129227
H78	13.5793913582	8.7394142769	20.9878310167
N79	11.3723799461	4.6387498121	12.8608021124
C80	10.0811208929	4.2354113403	13.0112585009
C81	11.6334734201	5.9599646270	12.6617272249
C82	12.4908102093	3.6924679679	13.0742272457
H83	9.9310186766	3.1771212720	13.1746190691
C84	9.0403326733	5.1151681054	12.9663304040
C85	10.6418049268	6.8919568244	12.6298056141
H86	12.6705043014	6.2247558907	12.5163023918
C87	12.9494283654	3.7610857516	14.5245046880
H88	13.2906865094	3.9738950366	12.3909257707
H89	12.1362286707	2.6976520143	12.8125503319
H90	8.0467911997	4.7173242928	13.1075006721
C91	9.2699294376	6.5190233303	12.7962655218
H92	10.9294601785	7.9162853244	12.4465906609
C93	12.4900647280	2.8424322960	15.4703134777
C94	13.7540233035	4.8217115857	14.9423193619
C95	8.2167831240	7.4746898399	12.7981877633
C96	12.8053969862	3.0103643118	16.8196224345
H97	11.8813395337	2.0004649740	15.1583586435
H98	14.1405584754	5.5241698393	14.2140083111

C99	14.0416739748	5.0069912102	16.2909546080
C100	6.8356194433	7.1005981226	12.7395769919
C101	8.4571840416	8.8866347193	12.8714842020
C102	13.5596123239	4.1086015379	17.2437168764
H103	12.4468644544	2.2879907864	17.5449964209
H104	14.6069588759	5.8733878557	16.6157582889
H105	6.5364876210	6.0741469644	12.5904109882
C106	5.8500607489	8.0341162942	12.8380577433
C107	7.4286488607	9.7666007026	13.0025240378
H108	9.4588531750	9.2884411260	12.8911878513
C109	13.7803316361	4.4040472437	18.7242760339
N110	6.1263843640	9.3591321553	13.0038543958
H111	4.8026060650	7.7712440314	12.7826426841
H112	7.5915572936	10.8288311156	13.1254380743
N113	12.7102072880	5.2249281904	19.2782451091
H114	13.8329958730	3.4725571067	19.2904817718
H115	14.7093797030	4.9576347168	18.8499485210
C116	5.0798261275	10.2768906080	13.4960072281
C117	12.7519424735	6.6019085149	19.0755051419
C118	11.4549483033	4.6494856591	19.4329312948
H119	4.1259973428	9.9316647369	13.0999167222
H120	5.2873535248	11.2726356457	13.1083961184
C121	5.0973519002	10.2568846151	15.0215602396
C122	11.6558413088	7.3777289273	19.1196656400
H123	13.7412929564	7.0025934208	18.8935442258
H124	11.4569356075	3.5728303353	19.5551996862
C125	10.3209901254	5.3629227465	19.4758471506

C126	5.4981344956	11.3628894234	15.7666155984
C127	4.8015717298	9.0614918231	15.6856748449
C128	10.3078137322	6.8257975680	19.3360090140
H129	11.7939482376	8.4409954173	18.9819583226
H130	9.3988565831	4.8263110155	19.6483152894
H131	5.7330753603	12.2979173168	15.2685853916
C132	5.6082233358	11.2684189429	17.1593713064
C133	4.9353949436	8.9590213586	17.0624258002
H134	4.4897350748	8.1932174352	15.1190113636
C135	9.1678968432	7.5657582222	19.3963960396
H136	5.9204086813	12.1366941656	17.7303252900
C137	5.3406160829	10.0671754694	17.8139267129
H138	4.7671886092	8.0045177887	17.5522749601
C139	9.1361686770	9.0317474836	19.2955419451
C140	7.8233792957	6.9940932618	19.5716726093
C141	5.5511593062	9.8938208587	19.3170271804
C142	7.9941722392	9.7314768644	19.3908352080
H143	10.0534310898	9.5856307860	19.1542524586
H144	7.6874201726	5.9239634528	19.6243373768
C145	6.7185643951	7.7550842147	19.6589977914
N146	6.7603525018	9.1409375291	19.6165828169
H147	4.7137272835	9.3416303274	19.7413425508
H148	5.6118667611	10.8714143518	19.7989201763
H149	7.9779541308	10.8126333582	19.3170943948
H150	5.7317366609	7.3274197117	19.7861909917

2⁰ CBPQT circling BQ

-3452.374194 -3452.318587 -3453.295585 -3453.351192

C1	10.4365455507	9.3289710098	20.3689468460
C2	9.0576767217	9.8461666408	20.3716193727
C3	10.9397346839	9.0943620977	21.7316525860
C4	11.1672267959	9.1143932337	19.2401667523
C5	8.3908736808	10.1052257006	21.5072243543
C6	10.2180886145	9.3905394095	22.8237510863
C7	12.5409755645	8.5823812148	19.2360384698
C8	10.6862551308	9.4179644424	17.8834581145
N9	8.9473872544	9.9558106483	22.7735419432
C10	13.2555447751	8.4618208737	18.1049484733
C11	11.4638981906	9.2779803018	16.7989634450
N12	12.7864396128	8.8564347503	16.8592188874
C13	7.4595565633	8.3319047230	23.8860186417
C14	8.2632711091	7.2519062310	24.2588177683
C15	6.1784501538	8.0819699023	23.3967194116
C16	12.9095760192	6.8802771072	15.3834927187
C17	7.8194144507	5.9443251751	24.1072773997
C18	5.7179383143	6.7698506114	23.2692485827
C19	13.6260129458	5.7643177177	15.8180603568
C20	11.6654528718	6.6910554139	14.7805210735
C21	6.5379413758	5.6941236493	23.6096248857
C22	13.0955104130	4.4822354580	15.6641982667
C23	11.1246634293	5.4178096043	14.6462141009
C24	6.1028915885	4.2559873972	23.3555995790
C25	11.8374290366	4.3011459819	15.0870449024
N26	6.6656404588	3.7344066513	22.1195044983

C27	11.1949671178	2.9226034354	14.9772133572
C28	7.9352104203	3.1706381433	22.1283997814
C29	6.1634718542	4.1621977296	20.8991042522
N30	10.2793472109	2.6303403687	16.0740508839
C31	8.6309928693	2.9551012819	21.0024242032
C32	6.7991162283	3.9620009542	19.7336746423
C33	9.0191868290	3.2267311283	16.0606777256
C34	10.8105259624	2.3161698585	17.3191263416
C35	8.1200020834	3.3160497849	19.6716265682
C36	8.3051503153	3.4381905474	17.1765014061
C37	10.1417226228	2.4876227026	18.4694697445
C38	8.8023111433	3.0936293120	18.5158004762
O39	10.2111142095	5.8229811967	22.0738413355
C40	11.4690392308	5.3282158373	22.4577934131
C41	9.9801645640	6.0042501150	20.7362442820
C42	11.5163853350	5.2846621383	23.9767040895
C43	10.9053210188	5.7018397229	19.7338313966
C44	8.7400189747	6.5262426408	20.3905230084
O45	10.7058513128	4.2202411250	24.4388155405
C46	10.5868259312	5.9253901192	18.4003929442
C47	8.4204373199	6.7475211323	19.0554623170
C48	10.6293323659	4.1535477304	25.8481687304
C49	9.3449434964	6.4451567026	18.0538893001
C50	10.1274317772	2.7771046610	26.2522578814
O51	9.1230000648	6.6350819036	16.7153395341
O52	8.7743966042	2.6074897077	25.8706836948
C53	7.8503721151	7.0720090835	16.3133374761

C54	8.3281399596	1.2968305528	26.1699191566
C55	7.8341937282	7.1628277970	14.7941711225
C56	6.8620472023	1.1294114341	25.8064681749
O57	7.8122179253	5.8613232703	14.2379342122
O58	6.7155072099	1.1289538031	24.4004709974
C59	7.7751154444	5.8657442517	12.8249413879
C60	5.4658096623	0.6120250321	23.9892848220
C61	7.5839086824	4.4384436323	12.3324829058
C62	5.2836507988	0.8319228606	22.4968937764
O63	8.7698841936	3.7003393620	12.5617789879
O64	6.2788580855	0.1017711116	21.8007130484
C65	8.7932345687	2.4266498619	11.9406710686
C66	6.3621012818	0.2945436367	20.4497444215
C67	7.5738396829	1.5642925793	12.2658866236
C68	5.4310462000	0.9963366756	19.6990386495
C69	7.4620976031	-0.2895253225	19.8048026965
O70	7.3937908562	1.5540149360	13.6653064685
C71	5.5794411658	1.1057225277	18.3089291682
C72	7.6023210507	-0.1923739204	18.4346116979
C73	6.1898792939	0.9270645144	14.0564672495
C74	6.6519109439	0.4993456942	17.6706036434
C75	5.9146874826	1.2067789659	15.5244155078
O76	6.8427763602	0.4904616622	16.3156248478
H77	8.5374398749	10.0166501735	19.4400936422
H78	11.9290279238	8.6879661720	21.8860161727
H79	7.3718883978	10.4724188166	21.4978782324
H80	10.6093516776	9.2340039548	23.8210642892

H81	13.0094885810	8.2669457726	20.1567813410
H82	9.6785599875	9.7754833663	17.7284908866
H83	14.2633364220	8.0656796063	18.1077015397
H84	11.1022502010	9.5175591213	15.8073851135
H85	9.2548093879	7.4378800402	24.6520959730
H86	5.5376698025	8.9092166004	23.1093500829
H87	8.4823188951	5.1163507097	24.3368399968
H88	4.7178824150	6.5861162059	22.8906431657
H89	14.5997759335	5.8940359135	16.2788323995
H90	11.1072713749	7.5489861002	14.4263338194
H91	13.6650691421	3.6218379155	15.9995070332
H92	10.1334633079	5.2865821337	14.2263908541
H93	6.4429689536	3.6032088105	24.1600908873
H94	5.0131809028	4.2010329536	23.2950127267
H95	10.6189724930	2.8751001367	14.0546965451
H96	11.9663881252	2.1511375528	14.9572300630
H97	8.3110751326	2.8967182007	23.1058200752
H98	5.1960698959	4.6478798810	20.9501453898
H99	9.6009698748	2.4929670451	21.1053496928
H100	6.3132026125	4.3016491881	18.8302543118
H101	8.6475281307	3.4907069240	15.0784823743
H102	11.8058165969	1.8868144331	17.2951773579
H103	7.3292850713	3.8878238732	17.0585395786
H104	10.6290460792	2.1731209550	19.3815491508
H105	11.6313993962	4.3218790821	22.0612138778
H106	12.2681910259	5.9876024306	22.1028092863
H107	12.5517838377	5.1300689630	24.3001873296

H108	11.1648384667	6.2434578957	24.3683793505
H109	11.8758174795	5.2916240652	19.9767039146
H110	8.0342192993	6.7499519260	21.1811519908
H111	11.2901639973	5.6938245651	17.6098073351
H112	7.4454848498	7.1476709193	18.8116036547
H113	11.6218465827	4.2907199470	26.2909834145
H114	9.9627152724	4.9302469539	26.2355136085
H115	10.7542952961	2.0220518669	25.7697543871
H116	10.2254194783	2.6718868669	27.3386342045
H117	7.0754438191	6.3742122340	16.6425419063
H118	7.6343215496	8.0653702999	16.7213887434
H119	8.9172902964	0.5621518969	25.6148547412
H120	8.4404930574	1.1026681141	27.2428466261
H121	6.9405301920	7.7151750566	14.4824404765
H122	8.7201094896	7.7109887585	14.4609629561
H123	6.2689820605	1.9338028155	26.2536786358
H124	6.5245148880	0.1741479975	26.2227268959
H125	6.9326952490	6.4701191098	12.4700824855
H126	8.7022359861	6.2792732981	12.4144005533
H127	5.4069514326	-0.4563212551	24.2220324597
H128	4.6479048949	1.1280266415	24.5048263585
H129	6.7474616538	3.9908724217	12.8752872250
H130	7.3539106735	4.4634762339	11.2613424242
H131	4.2866048824	0.4791063696	22.2159709525
H132	5.3883715010	1.8920823841	22.2679287823
H133	8.8593306705	2.5331670530	10.8523568288
H134	9.6919767311	1.9306129386	12.3015722297

H135	7.7503005253	0.5545805779	11.8790942675
H136	6.6803019739	1.9627838308	11.7740708772
H137	4.5883686148	1.4839412930	20.1686355297
H138	8.1947387335	-0.8136961647	20.4049308624
H139	4.8468347769	1.6762724467	17.7549751450
H140	8.4510163419	-0.6346549595	17.9302271899
H141	5.3517651957	1.3313470968	13.4779609690
H142	6.2413205393	-0.1537638213	13.8886283879
H143	4.8964710745	0.8733269874	15.7442543501
H144	6.0054792649	2.2771421230	15.7171100214
C145	8.0419139540	9.7399087078	23.9050695794
H146	8.6085028438	9.9065093136	24.8218473017
H147	7.2461414857	10.4831106089	23.8512635884
C148	13.4045349100	8.2956238166	15.6560594213
H149	13.1582617271	8.9493623734	14.8181639409
H150	14.4860809313	8.3052670328	15.7937853914

2⁴⁺ CBPQT circling glycol chain

-3451.817540 -3451.113300 -3452.064319 -3452.768559

O1	24.9035691394	11.3130056851	20.5497214771
C2	24.1003002645	12.3358544713	20.9453595488
C3	25.7988406337	11.5247939133	19.4648930594
C4	23.1697427558	12.0266682682	21.9508799007
C5	24.1487575316	13.6263742506	20.4323728375
H6	26.5068384003	12.3186434202	19.7092120639
H7	25.2405639072	11.7907269835	18.5646577334
C8	26.5670695562	10.2316879112	19.2360816873

C9	22.3058393341	12.9935018862	22.4267873681
H10	23.1420216306	11.0166027175	22.3392628859
H11	24.8453024234	13.8925157574	19.6488585908
C12	23.2756019636	14.6100197024	20.9217991597
O13	27.4548638452	10.0523423940	20.3212528670
H14	25.8661091302	9.3950065430	19.1595074384
H15	27.1206540076	10.3181009433	18.2961140614
C16	22.3528532735	14.2959150693	21.9090014425
H17	21.5783623992	12.7597852246	23.1940784145
H18	23.3387787299	15.6072814153	20.5098430951
C19	28.2633170602	8.8942403815	20.2107907438
O20	21.4752715129	15.1961955070	22.4675589075
H21	28.8713004404	8.9368810001	19.3023102588
H22	27.6374788077	7.9970067684	20.1759630155
C23	29.1736176524	8.8091021889	21.4283562797
C24	21.4053086356	16.4919824111	21.8973964711
O25	30.1388372460	9.8435830030	21.3632334040
H26	28.5745995083	8.9010952283	22.3389960835
H27	29.6650932551	7.8308547852	21.4292662917
C28	20.2512130361	17.2349648503	22.5988401465
H29	21.2107224646	16.4128289653	20.8263883564
H30	22.3493300014	17.0260051656	22.0525508443
C31	31.0633833037	9.8044277636	22.4357958717
O32	20.4826538294	18.6358986042	22.5998947392
H33	19.3128218429	17.0597113990	22.0784822867
H34	20.1552485513	16.8603529215	23.6218307370
H35	31.5653154406	8.8319144251	22.4693967930

H36	30.5502056644	9.9672205019	23.3882377857
C37	32.1167262494	10.8848713215	22.2329231853
C38	21.3790893670	19.0333366792	23.6215519493
O39	31.5083669317	12.1576628614	22.3663703752
H40	32.8979974726	10.7555427495	22.9885881748
H41	32.5654082305	10.7780136626	21.2405376843
C42	21.8224771143	20.4636177328	23.3412043986
H43	22.2681608771	18.3979500870	23.6299906774
H44	20.8950691662	18.9683403314	24.6007457266
C45	32.4230819440	13.2310066982	22.2553127175
O46	22.9562624025	20.7172887892	24.1392380596
H47	22.0694900214	20.5440368856	22.2773590684
H48	21.0149556763	21.1643608493	23.5718091260
H49	32.9394850055	13.2005068862	21.2909848812
H50	33.1681542329	13.1909841784	23.0559036526
C51	31.6455830106	14.5357685537	22.3446200212
C52	23.4064250331	22.0608397098	24.0454908173
O53	31.1540238795	14.6573833603	23.6726396328
H54	32.3038519939	15.3743771248	22.1075394325
H55	30.8147435231	14.5091129423	21.6386999204
C56	24.6412742401	22.2174091359	24.9172738821
H57	22.6274858641	22.7457329917	24.3905096428
H58	23.6576822160	22.3006855190	23.0070510456
C59	30.3170146651	15.6885852586	23.9715230152
O60	25.7010821034	21.4396570185	24.3760117676
H61	24.9344267607	23.2685284760	24.9413131762
H62	24.4044260440	21.8944063696	25.9324876862

C63	29.9308066703	16.6824645380	23.0779023695
C64	29.8316691238	15.7147530186	25.2875237045
C65	26.2849595944	20.5343662085	25.2758294383
H66	30.3071583231	16.7000183217	22.0642477264
C67	29.0393000826	17.6861145429	23.4836800849
C68	28.9597081872	16.7094203489	25.6903633922
H69	30.1509861132	14.9421158880	25.9754176346
C70	27.3775864319	19.7766293581	24.5197058722
H71	25.5394740094	19.8267120425	25.6219535030
H72	26.6959324407	21.0473203264	26.1373200957
H73	28.7491475300	18.4457298116	22.7702720971
C74	28.5460020313	17.6927180452	24.7818569144
H75	28.5827337497	16.7402289500	26.7060740771
O76	27.5938254732	18.5709826035	25.2449640583
H77	27.0152691175	19.5610159259	23.5147124657
H78	28.3014163343	20.3537840500	24.4622132062
N79	23.5659767399	19.8198838680	19.3086947744
C80	23.2567168664	21.1200191332	19.4134736918
C81	22.6035217869	18.8795487848	19.2948792810
C82	24.9887274559	19.3642576115	19.3353048303
H83	24.0724183823	21.8275221596	19.3520596823
C84	21.9446271711	21.5200609540	19.6275127171
C85	21.2869242306	19.2141188585	19.5214967913
H86	22.9261982908	17.8601292700	19.1317382983
C87	25.2125754349	18.5555732805	20.6137995346
H88	25.6128586558	20.2539128717	19.2962773195
H89	25.1629459329	18.7598697829	18.4476668188

H90	21.7413211081	22.5788213338	19.7166348104
C91	20.9489652131	20.5520208073	19.7622181954
H92	20.5524652798	18.4220310146	19.5532852001
C93	25.8390162329	17.3118559483	20.5530703282
C94	24.7704434041	19.0306566545	21.8521046122
C95	19.5914779976	20.8750582824	20.3031336864
C96	25.9958640986	16.5432711066	21.7082544045
H97	26.1963582018	16.9330931853	19.6032677245
H98	24.3160436184	20.0103317019	21.9502559310
C99	24.9147041772	18.2575964586	23.0013793065
C100	19.4371268083	21.9508938226	21.1850666883
C101	18.4925842039	20.0490360198	20.0615637982
C102	25.5197048053	16.9983855752	22.9365231305
H103	26.4728410738	15.5731088664	21.6421665569
H104	24.5478888310	18.6718468210	23.9345123016
H105	20.2344931485	22.6516264141	21.3898725981
C106	18.2488226074	22.1009034547	21.8714936438
C107	17.3255423089	20.2473806607	20.7796261155
H108	18.5170697885	19.2428669756	19.3412516824
C109	25.6998307903	16.1125331233	24.1677990381
N110	17.2401503620	21.2322113862	21.6875569388
H111	18.0896781545	22.8874342600	22.5968890935
H112	16.4586825731	19.6117733999	20.6606932342
N113	24.5752195707	16.3127311554	25.1168667273
H114	25.6988831119	15.0610141290	23.8907187542
H115	26.6224112186	16.3405252801	24.6953194676
C116	16.0734634718	21.3010252204	22.6037800343

C117	23.4033536720	15.7239319613	24.8295851134
C118	24.7092824035	17.1230561770	26.1790640796
H119	15.2590692726	20.7501695548	22.1376323732
H120	15.7903919932	22.3470589145	22.7007303625
C121	16.4441050868	20.6991930625	23.9610622255
C122	22.2810737730	15.9898035570	25.5837500201
H123	23.3924382376	15.0561927269	23.9789874324
H124	25.6980598213	17.5283416334	26.3583357071
C125	23.6127510576	17.4393268578	26.9688614401
C126	15.6639067329	21.0316049708	25.0733205111
C127	17.5053677394	19.8125278473	24.1220232453
C128	22.3656886992	16.8987387689	26.6456104099
H129	21.3532386993	15.5107226979	25.3026808550
H130	23.7546444355	18.0961610251	27.8168129319
H131	14.8396327740	21.7276115360	24.9674114765
C132	15.9420825378	20.4862364984	26.3226225474
C133	17.7755760079	19.2593108812	25.3743347754
H134	18.1483175572	19.5369667668	23.2931993867
C135	21.0932728436	17.3612273138	27.2841218313
H136	15.3329416843	20.7662160778	27.1744124576
C137	17.0045593572	19.5914816129	26.4849234939
H138	18.5988372467	18.5597175474	25.4554725426
C139	19.9836483415	16.5179800252	27.3795404146
C140	20.9477262195	18.7068017231	27.6414375234
C141	17.2686942426	19.0083355936	27.8778293174
C142	18.7456110310	17.0664072184	27.6742824431
H143	20.0439870513	15.4549110748	27.1896679260

H144	21.7762272471	19.4014619687	27.6270649542
C145	19.6894193171	19.1932972783	27.9384613220
N146	18.6166558452	18.3847386295	27.8922189652
H147	17.2509646638	19.7863638748	28.6382319653
H148	16.5438053866	18.2378209880	28.1316804417
H149	17.8406742988	16.4747882610	27.6915211334
H150	19.5063715278	20.2358235461	28.1613142725

2³⁺ CBPQT circling glycol chain

-3451.979604 -3451.544953 -3452.501423 -3452.936074

O1	24.7525504923	11.5235480797	20.8998544749
C2	23.9178343975	12.5395042743	21.2568847222
C3	25.7521174390	11.7828677823	19.9206748394
C4	22.8169776147	12.1841214717	22.0542311463
C5	24.0894452286	13.8674103092	20.8866926156
H6	26.4705702514	12.5164493838	20.2933978511
H7	25.2850949705	12.1526930504	19.0052776511
C8	26.4853816803	10.4803564450	19.6361825899
C9	21.9072521906	13.1428424166	22.4601778300
H10	22.6931156287	11.1460000938	22.3362629247
H11	24.9172524944	14.1718241041	20.2617322440
C12	23.1747833890	14.8427829505	21.3110722269
O13	27.3152951454	10.1880202985	20.7417361796
H14	25.7588452669	9.6799332158	19.4652579358
H15	27.0862230188	10.6107528831	18.7312474942
C16	22.0827824309	14.4847211205	22.0895710257
H17	21.0526047996	12.8744204644	23.0689128976

H18	23.3488767654	15.8698509350	21.0212558049
C19	28.0902414197	9.0131777885	20.5738996741
O20	21.1480969861	15.3676237469	22.5586831199
H21	28.6498471760	9.0551514956	19.6346827755
H22	27.4432863272	8.1307827977	20.5613800404
C23	29.0716610065	8.9015609878	21.7327282802
C24	21.3695289401	16.7411694223	22.3044160899
O25	30.0688864850	9.8947252096	21.5794532752
H26	28.5372527105	9.0329671458	22.6786422684
H27	29.5222671576	7.9039254530	21.7194607719
C28	20.2881532116	17.5210253674	23.0587908128
H29	21.2941807188	16.9418689244	21.2342684678
H30	22.3632204022	17.0306553076	22.6554454179
C31	31.0654764261	9.8535779908	22.5848022755
O32	20.5596088882	18.9131332954	22.9859144703
H33	19.3132152871	17.3480760184	22.6065190121
H34	20.2643400484	17.1852959500	24.0980634040
H35	31.5379675158	8.8663354015	22.6158166467
H36	30.6283503111	10.0664580247	23.5652821477
C37	32.1290468479	10.8955295793	22.2656967785
C38	21.5155396861	19.3392508119	23.9462060306
O39	31.5469520319	12.1822319145	22.3638504965
H40	32.9502462040	10.7892840490	22.9817005810
H41	32.5170859732	10.7279097019	21.2563071729
C42	22.0015817081	20.7255809493	23.5361127761
H43	22.3754677965	18.6672468336	23.9663403203
H44	21.0746733889	19.3638827626	24.9459209948

C45	32.4640749696	13.2387138124	22.1626841971
O46	23.2112692061	20.9739875981	24.2197021529
H47	22.1592441987	20.7260621764	22.4513676478
H48	21.2517901585	21.4826106730	23.7861167547
H49	32.9481169004	13.1503746401	21.1852509040
H50	33.2344154780	13.2391509758	22.9399932026
C51	31.6908058819	14.5485449275	22.2048242779
C52	23.6854940988	22.2978909287	24.0230811904
O53	31.2415200995	14.7402432435	23.5393525695
H54	32.3400177948	15.3729600451	21.9014312816
H55	30.8382657797	14.4828995813	21.5271398434
C56	24.9456250223	22.5261324686	24.8470975216
H57	22.9243504862	23.0185182962	24.3367989234
H58	23.9149721796	22.4599352704	22.9645662855
C59	30.3759989402	15.7582215794	23.8018986497
O60	26.0379665225	21.7728380212	24.3424511169
H61	25.2093257591	23.5818744604	24.7790474095
H62	24.7543144255	22.2794905384	25.8937141867
C63	29.9431574933	16.6951861166	22.8685188801
C64	29.9151342401	15.8360247807	25.1246569887
C65	26.3106284458	20.5845380268	25.0598540196
H66	30.3005538299	16.6730982831	21.8478856435
C67	29.0259031089	17.6889650738	23.2423367252
C68	29.0177853872	16.8207830262	25.4943586809
H69	30.2730488039	15.1095397696	25.8430479029
C70	27.3704331927	19.8203246552	24.2696200612
H71	25.4077119155	19.9786822738	25.1502583415

H72	26.6896096339	20.8138571642	26.0589630011
H73	28.6909313780	18.3996798499	22.4983050400
C74	28.5527746988	17.7427432165	24.5464923449
H75	28.6536458100	16.8883083285	26.5128138163
O76	27.5818904493	18.6095585983	24.9840791200
H77	26.9965908164	19.6213557638	23.2649996527
H78	28.2981655399	20.3928512863	24.2137671736
N79	23.5739769985	19.7681294851	19.2999578741
C80	23.3061767968	21.0708789293	19.4740086234
C81	22.5858467710	18.8560704042	19.2742036302
C82	24.9822719957	19.2764813539	19.2638872731
H83	24.1418071179	21.7556632707	19.4258143194
C84	22.0120490947	21.4996076652	19.7319902743
C85	21.2831100628	19.2210042957	19.5382710733
H86	22.8747341364	17.8330659660	19.0711127624
C87	25.2450824739	18.4586224238	20.5286694325
H88	25.6268232269	20.1490995733	19.1943939047
H89	25.0996290700	18.6688235195	18.3691859554
H90	21.8443940610	22.5593322737	19.8684484586
C91	20.9864756731	20.5576787962	19.8348228975
H92	20.5287226856	18.4473200343	19.5478265829
C93	26.0017168224	17.2869647208	20.4537678815
C94	24.7296402484	18.8509063806	21.7659652288
C95	19.6333192897	20.9091522199	20.3702897511
C96	26.2076592847	16.5056860626	21.5916666360
H97	26.4194624930	16.9738443451	19.5040400210
H98	24.1732383585	19.7761616731	21.8789880939

C99	24.9169295257	18.0538212584	22.8925076847
C100	19.4796055584	22.0087191790	21.2206593609
C101	18.5259648836	20.0889008331	20.1370841356
C102	25.6393045588	16.8618872742	22.8163750256
H103	26.7968517703	15.5990687565	21.5148449356
H104	24.4812946363	18.3809345583	23.8277402385
H105	20.2797355791	22.7055761699	21.4213049298
C106	18.2814131638	22.1958756357	21.8821857606
C107	17.3557220955	20.3155184787	20.8400276515
H108	18.5470920201	19.2656497661	19.4377395323
C109	25.8169733678	15.9447898609	24.0283856073
N110	17.2669513254	21.3316912696	21.7134342797
H111	18.1226134598	23.0049945305	22.5822855571
H112	16.4883746178	19.6767312992	20.7406470434
N113	24.6873905427	16.0578986029	24.9574118193
H114	25.8733936859	14.9100491963	23.6994520384
H115	26.7295913599	16.1914187280	24.5657878335
C116	16.1076476792	21.4070886164	22.6350981367
C117	23.5954307880	15.2621027531	24.7854855034
C118	24.6468800477	17.0544043241	25.8879262404
H119	15.2548618289	20.9577282377	22.1307661988
H120	15.9012785739	22.4591900113	22.8222752701
C121	16.4407077455	20.6654750842	23.9322331689
C122	22.4285426333	15.4887705826	25.4503008400
H123	23.7136393024	14.4433456210	24.0894854744
H124	25.5699419438	17.6048967543	26.0238115148
C125	23.5054351484	17.3436384672	26.5772535684

C126	15.4896936677	20.6719251044	24.9606754647
C127	17.6373012487	19.9839640623	24.1243894189
C128	22.2961013375	16.6024433208	26.3448398985
H129	21.6093984691	14.8141425658	25.2540185277
H130	23.5517395304	18.1434299088	27.3015614133
H131	14.5518964586	21.1995516856	24.8268687023
C132	15.7364557594	20.0062985219	26.1553681046
C133	17.8802196379	19.3171388467	25.3272927849
H134	18.4120135299	19.9430164366	23.3655254139
C135	21.0410721503	16.9711504390	26.9083787033
H136	14.9882522695	20.0223356189	26.9401528176
C137	16.9399900985	19.3176503939	26.3510454865
H138	18.8202740130	18.7941059674	25.4415153980
C139	19.8423671547	16.2121703353	26.6867593117
C140	20.8615000327	18.1723947937	27.6713817090
C141	17.1872676486	18.5884408053	27.6764745111
C142	18.6241295005	16.7088558826	27.0434944309
H143	19.8601813272	15.2394291869	26.2190312177
H144	21.6966724011	18.7837716453	27.9779432313
C145	19.6146884965	18.6178784970	27.9948641751
N146	18.4942609537	17.9223227115	27.6517154228
H147	17.1790378661	19.2928754698	28.5072831455
H148	16.4195809862	17.8347632322	27.8473779482
H149	17.7038175222	16.1770341773	26.8413455683
H150	19.4548976601	19.5525200102	28.5158828095

2²⁺ CBPQT circling glycol chain

-3452.138738 -3451.919671 -3452.880485 -3453.099552

O1	24.7200472822	11.5377436444	20.9014824304
C2	23.8746112714	12.5545610188	21.2329796541
C3	25.7185095482	11.7735165880	19.9170468165
C4	22.7718718476	12.1966438949	22.0251499480
C5	24.0359750183	13.8799843848	20.8468033912
H6	26.4422231683	12.5093380886	20.2751304027
H7	25.2537136665	12.1285399496	18.9946957481
C8	26.4396370856	10.4582597146	19.6592265186
C9	21.8530448991	13.1519446737	22.4154776918
H10	22.6554332692	11.1602343981	22.3167342119
H11	24.8660140279	14.1836775103	20.2238245637
C12	23.1101682078	14.8543285418	21.2543647319
O13	27.2656953124	10.1781778952	20.7712868152
H14	25.7035775377	9.6632121293	19.5045141783
H15	27.0427304841	10.5626128799	18.7523697801
C16	22.0203418505	14.4923823959	22.0356770950
H17	20.9963908319	12.8838902161	23.0216385385
H18	23.2693118063	15.8812919034	20.9499676457
C19	28.0150345606	8.9831564318	20.6327147993
O20	21.0737448567	15.3613753310	22.4992306787
H21	28.5603710925	8.9820550429	19.6843321374
H22	27.3520383569	8.1129621966	20.6605023659
C23	29.0137825812	8.8943638664	21.7786328657
C24	21.2911841013	16.7498271663	22.3135843490
O25	30.0081849175	9.8826366006	21.5836944999
H26	28.4957752895	9.0514349351	22.7297614131

H27	29.4613719853	7.8952606809	21.7829233083
C28	20.2576771573	17.4647767666	23.1895407790
H29	21.1546928330	17.0280758890	21.2667014701
H30	22.3047722800	17.0132586391	22.6258182403
C31	31.0193518842	9.8761589613	22.5742872441
O32	20.4761094599	18.8622877398	23.1624437280
H33	19.2551491905	17.2830289089	22.8053702438
H34	20.3249505843	17.0773731600	24.2094985533
H35	31.5236731854	8.9047314740	22.6016213089
H36	30.5912235525	10.0776988735	23.5608025562
C37	32.0417245140	10.9525475700	22.2340310376
C38	21.5075492923	19.3017269110	24.0285915268
O39	31.4182814551	12.2192058938	22.3437458660
H40	32.8811295274	10.8761242416	22.9324381806
H41	32.4137482905	10.7970969438	21.2166760994
C42	21.9535831973	20.6713695050	23.5339079793
H43	22.3614334155	18.6223446374	23.9973699777
H44	21.1515848462	19.3600887983	25.0605768119
C45	32.2914501905	13.3055248187	22.1084572163
O46	23.1351920429	21.0109343587	24.2320829337
H47	22.1378091838	20.6062959545	22.4581693148
H48	21.1662837101	21.4105039658	23.7149738839
H49	32.7476478886	13.2264381713	21.1168085193
H50	33.0854517273	13.3376412969	22.8609083190
C51	31.4782558145	14.5906541895	22.1653886253
C52	23.5982648873	22.3150661311	23.9239426398
O53	31.0674788980	14.7860718131	23.5116873995

H54	32.0921865286	15.4303011712	21.8318283808
H55	30.6051467667	14.4929230597	21.5180020284
C56	24.8385716831	22.6232436175	24.7523921977
H57	22.8233313582	23.0529335686	24.1546753195
H58	23.8504152866	22.3847872432	22.8613819095
C59	30.2172318563	15.8127884115	23.7941442782
O60	25.9563852752	21.8587596136	24.3259805750
H61	25.0915164820	23.6739990494	24.6106771627
H62	24.6314250731	22.4493874732	25.8106614089
C63	29.7574682135	16.7410048628	22.8651093927
C64	29.8053721354	15.9126353021	25.1317755382
C65	26.1700543229	20.6599609498	25.0482533618
H66	30.0755492721	16.7025122001	21.8319412541
C67	28.8626624155	17.7470614154	23.2581221120
C68	28.9273293409	16.9086313544	25.5197474446
H69	30.1853996004	15.1947907258	25.8475516842
C70	27.2581839317	19.8962730709	24.2978797195
H71	25.2560812578	20.0655201746	25.0860695215
H72	26.5032745025	20.8768026917	26.0666206195
H73	28.5062096926	18.4480026585	22.5149696186
C74	28.4327379674	17.8199740655	24.5763292600
H75	28.6005349322	16.9928430741	26.5494074252
O76	27.4843968169	18.7000183597	25.0335954012
H77	26.9043078892	19.6752186688	23.2913896047
H78	28.1765490359	20.4847263734	24.2475496337
N79	23.7821995027	19.8827544728	19.3152360611
C80	23.4713234652	21.1434883268	19.7304708053

C81	22.7728710996	18.9901023403	19.0909185830
C82	25.1676591518	19.3890820897	19.3292641165
H83	24.3005545051	21.8321798875	19.8237123517
C84	22.1886705825	21.5095440649	20.0164916050
C85	21.4748189559	19.2945986601	19.3550339262
H86	23.0718500876	18.0267379848	18.6989524277
C87	25.3708616026	18.4859373261	20.5477736962
H88	25.8301733816	20.2527540413	19.3590934601
H89	25.3522330584	18.8367313632	18.4088650425
H90	22.0243096648	22.5299499066	20.3306514005
C91	21.1141071941	20.5613033298	19.9258040004
H92	20.7347200811	18.5391909902	19.1361301829
C93	26.1161890092	17.3091761173	20.4472266590
C94	24.7925672168	18.8118987388	21.7757266477
C95	19.8081652089	20.8211150235	20.4273501071
C96	26.2661486331	16.4702882314	21.5515382513
H97	26.5716297241	17.0397881729	19.5010636818
H98	24.2195679808	19.7257481608	21.8974785965
C99	24.9400498668	17.9679073559	22.8738599595
C100	19.4734813844	22.0408450616	21.0996159554
C101	18.7497114032	19.8570744016	20.3545652388
C102	25.6652517979	16.7816371983	22.7725582411
H103	26.8490746710	15.5607883802	21.4583335466
H104	24.4760671775	18.2545867543	23.8086324679
H105	20.1737228256	22.8594569889	21.1750013190
C106	18.2639445385	22.1984773429	21.7088426570
C107	17.5551074211	20.0829133465	20.9712236073

H108	18.8614006994	18.9237889544	19.8237984318
C109	25.8272151908	15.8269417837	23.9554744335
N110	17.3113530085	21.2279971387	21.6690255521
H111	18.0113310797	23.0927120399	22.2628842875
H112	16.7519320906	19.3583579299	20.9546240069
N113	24.7188160524	15.9537187330	24.9081440114
H114	25.8350526802	14.8007524649	23.5971327345
H115	26.7604278078	16.0233869342	24.4809579117
C116	16.1568806520	21.2965567663	22.5737393766
C117	23.6077031145	15.1828610599	24.7494637548
C118	24.7089293907	16.9513304918	25.8383311419
H119	15.3179351592	20.7946660830	22.0926884121
H120	15.9002796867	22.3450305580	22.7188312211
C121	16.4874989339	20.6261896183	23.9110326455
C122	22.4565094646	15.4279983295	25.4343384837
H123	23.6936622073	14.3691086568	24.0440104733
H124	25.6368989824	17.4998228563	25.9518146578
C125	23.5839697763	17.2552736169	26.5476382508
C126	15.5298556710	20.6101305855	24.9333749534
C127	17.7140780781	20.0108217603	24.1310333604
C128	22.3563843610	16.5396842227	26.3342139506
H129	21.6192779793	14.7741021064	25.2415179108
H130	23.6543366373	18.0563642290	27.2688117895
H131	14.5691307889	21.0903439583	24.7818754960
C132	15.7957584512	19.9766140038	26.1431179319
C133	17.9758644986	19.3728437908	25.3444623291
H134	18.4932655648	19.9958652713	23.3775136831

C135	21.1146189338	16.9363337589	26.9093989783
H136	15.0400687199	19.9705503159	26.9213286178
C137	17.0261435688	19.3425165270	26.3586753576
H138	18.9380672492	18.8943910909	25.4708649949
C139	19.8992398264	16.1994808136	26.7046863373
C140	20.9639367216	18.1497931421	27.6590258318
C141	17.2929387110	18.6338000736	27.6914359944
C142	18.6933080282	16.7268270040	27.0588938568
H143	19.8949885953	15.2212205494	26.2479604237
H144	21.8138718077	18.7497684217	27.9484180966
C145	19.7276018192	18.6247301126	27.9829822821
N146	18.5911075576	17.9485168123	27.6548545315
H147	17.3116454966	19.3494526306	28.5118995023
H148	16.5200997879	17.8926997328	27.8915451069
H149	17.7609909746	16.2128952881	26.8663865850
H150	19.5900876196	19.5698120881	28.4911378058

2¹⁺ CBPQT circling glycol chain

-3452.269082 -3452.153287 -3453.123480 -3453.239274

O1	24.7227782513	11.5405764494	20.8804341920
C2	23.8681936129	12.5483066734	21.2265703830
C3	25.7431036366	11.8162754304	19.9301843706
C4	22.7490372801	12.1700254993	21.9836477596
C5	24.0416668798	13.8841214942	20.8848492864
H6	26.4564257929	12.5395061969	20.3317579529
H7	25.2982756023	12.2057542291	19.0115447357
C8	26.4763755429	10.5155492587	19.6366180538

C9	21.8247195535	13.1173710024	22.3836275365
H10	22.6248971259	11.1260600577	22.2435324847
H11	24.8889523493	14.2047600782	20.2952421328
C12	23.1107574991	14.8482417243	21.2999477518
O13	27.2840962860	10.1962092207	20.7517335553
H14	25.7477060877	9.7231336052	19.4389214698
H15	27.0952382971	10.6559317192	18.7453983089
C16	22.0022443218	14.4671978142	22.0455743702
H17	20.9575362070	12.8362264870	22.9684496578
H18	23.2812877563	15.8845656380	21.0362914210
C19	28.0363248505	9.0075835878	20.5805112533
O20	21.0419945116	15.3269520021	22.4931214996
H21	28.5808623227	9.0335848783	19.6318683915
H22	27.3750855110	8.1355609153	20.5848977434
C23	29.0366808524	8.8910708178	21.7226371650
C24	21.3174513913	16.7178569878	22.4391035916
O25	30.0305940567	9.8830100860	21.5473361730
H26	28.5195754254	9.0290386784	22.6772614972
H27	29.4845539177	7.8922917977	21.7056800772
C28	20.2814765257	17.4051716391	23.3313077742
H29	21.2288849994	17.0924560379	21.4164044102
H30	22.3259497944	16.9079495957	22.8108213058
C31	31.0356134007	9.8667543704	22.5431318286
O32	20.4863916063	18.8054293598	23.3017870947
H33	19.2796810323	17.2154384243	22.9465358556
H34	20.3596927456	17.0199344269	24.3497019417
H35	31.5505755751	8.9003187377	22.5537841534

H36	30.5991008534	10.0438914396	23.5303186051
C37	32.0467266991	10.9621382000	22.2305739002
C38	21.5042870948	19.2650386528	24.1782600456
O39	31.4068754807	12.2191746491	22.3585230999
H40	32.8832442605	10.8830563478	22.9323248022
H41	32.4267682860	10.8300784660	21.2128930228
C42	21.9689781139	20.6010573366	23.6141794871
H43	22.3458214754	18.5704162332	24.2080101989
H44	21.1210895498	19.3781046838	25.1953138333
C45	32.2659905119	13.3198632774	22.1387642082
O46	23.1284740036	21.0051399937	24.3150893148
H47	22.1831580514	20.4669281089	22.5495941654
H48	21.1721489235	21.3448273490	23.7219027430
H49	32.7321986910	13.2559989520	21.1507206361
H50	33.0531187469	13.3548694535	22.8984876169
C51	31.4372921880	14.5949648374	22.2019565322
C52	23.5841138517	22.2841512433	23.9122663622
O53	31.0074327940	14.7724378956	23.5440307642
H54	32.0449059780	15.4454539104	21.8840432548
H55	30.5730232762	14.4947999120	21.5440184023
C56	24.8326665846	22.6565486978	24.7012777783
H57	22.8077448768	23.0351213263	24.0939476749
H58	23.8283346444	22.2787020270	22.8450679547
C59	30.1735557402	15.8144300554	23.8268220372
O60	25.9573086542	21.8891692474	24.3009782086
H61	25.0673663719	23.7014488470	24.4967801976
H62	24.6454267666	22.5404521918	25.7713143184

C63	29.7248925392	16.7464197427	22.8975373999
C64	29.7669283304	15.9232121247	25.1651661489
C65	26.1610807724	20.6949469500	25.0374358786
H66	30.0330291707	16.6970616629	21.8618301031
C67	28.8503053325	17.7702068608	23.2912874686
C68	28.9087409657	16.9353131093	25.5535657422
H69	30.1346446182	15.1984812921	25.8806038363
C70	27.2418804403	19.9162882258	24.2924389401
H71	25.2440117307	20.1067057036	25.0857394277
H72	26.5013245577	20.9242458216	26.0510228522
H73	28.5007225544	18.4718543613	22.5458246888
C74	28.4286686772	17.8561215694	24.6110823889
H75	28.5839982764	17.0256952561	26.5832630056
O76	27.5180540287	18.7655542862	25.0783155678
H77	26.8625317482	19.6371626952	23.3099302780
H78	28.1447698764	20.5216665264	24.1837970364
N79	23.8666700378	19.7680619391	19.3399733036
C80	23.5782326575	21.0269931411	19.7773773256
C81	22.8419725050	18.8921866805	19.1183508596
C82	25.2427799378	19.2477738354	19.3624562882
H83	24.4183475206	21.7024927063	19.8695832629
C84	22.3048412676	21.4050373514	20.0892080669
C85	21.5511250116	19.2111245918	19.4018495231
H86	23.1239136431	17.9271866601	18.7179294909
C87	25.4225830761	18.3593259360	20.5949503812
H88	25.9210121758	20.0994246415	19.3793405840
H89	25.4169841723	18.6781354462	18.4506235394

H90	22.1555756330	22.4240472452	20.4150595008
C91	21.2164040968	20.4730155955	19.9993763451
H92	20.7992385857	18.4647643282	19.1912424433
C93	26.1691570161	17.1809859824	20.5243431507
C94	24.8168311789	18.6990182433	21.8059143147
C95	19.9230558858	20.7433253420	20.5261885557
C96	26.2956486043	16.3592728770	21.6436815509
H97	26.6428328821	16.8983620705	19.5908059827
H98	24.2411796427	19.6130590180	21.9019746911
C99	24.9344051338	17.8671621448	22.9168847703
C100	19.6313224293	21.9353106012	21.2651758607
C101	18.8357701496	19.8164606325	20.4120789405
C102	25.6662102280	16.6826668133	22.8471529191
H103	26.8817856779	15.4493867580	21.5763478445
H104	24.4410581239	18.1506761104	23.8390287402
H105	20.3652864027	22.7175426266	21.3939513046
C106	18.4260771776	22.1069367804	21.8786619976
C107	17.6457369190	20.0561951079	21.0326475923
H108	18.9183399261	18.9055581857	19.8385748832
C109	25.7910157996	15.7527309296	24.0545395664
N110	17.4354590148	21.1781699635	21.7761134175
H111	18.2040394078	22.9777146755	22.4812628935
H112	16.8173328178	19.3619422580	20.9772764942
N113	24.6975773501	15.8869503927	25.0022001370
H114	25.8031158173	14.7220041221	23.7038364951
H115	26.7324517646	15.9508332293	24.5675271649
C116	16.2548152965	21.2661662505	22.6446589277

C117	23.5424724058	15.1493869751	24.8197448593
C118	24.6393439663	16.9592689524	25.8747492415
H119	15.4217478470	20.7877579848	22.1307251839
H120	16.0165099965	22.3192973534	22.7874428772
C121	16.5269280594	20.5826112443	23.9866936583
C122	22.3849590583	15.4311038014	25.4433721275
H123	23.6374597233	14.3065189664	24.1475245548
H124	25.5695555476	17.5025450087	25.9942895481
C125	23.5108207410	17.3175846507	26.5181295679
C126	15.5424599220	20.5987741601	24.9831310895
C127	17.7289571706	19.9315793065	24.2382083309
C128	22.2381380005	16.5954042994	26.3331211111
H129	21.5488328375	14.7761456204	25.2458077903
H130	23.5717257372	18.1597332004	27.1931329471
H131	14.5987870695	21.1030257133	24.8033615782
C132	15.7647436744	19.9680065763	26.2033085990
C133	17.9467226150	19.2977227421	25.4628016018
H134	18.5231970556	19.8877638342	23.5025239675
C135	21.0539337561	16.9664715185	26.9000923815
H136	14.9915624462	19.9878018472	26.9645108676
C137	16.9738120098	19.3068748045	26.4556200181
H138	18.8885283201	18.7898109439	25.6255714749
C139	19.7947366221	16.2130810358	26.7345176788
C140	20.8733495734	18.1808415426	27.7175947948
C141	17.2147770405	18.6054759722	27.7968307148
C142	18.6138124525	16.6954910011	27.1595555264
H143	19.7932074794	15.2376636431	26.2688001411

H144	21.7237559786	18.7747427306	28.0196062744
C145	19.6555136511	18.6033756260	28.1046125884
N146	18.4878610810	17.9025987565	27.8334673843
H147	17.2036411315	19.3390551019	28.6041389984
H148	16.4132595568	17.8885315727	27.9838483489
H149	17.6873781762	16.1526903732	27.0158237197
H150	19.5207604809	19.5145814861	28.6746142106

2⁰ CBPQT circling glycol chain

-3452.394624 -3452.325341 -3453.305409 -3453.374692

O1 6.424035 1.074150 -5.287101

C2 5.199856 0.883213 -4.708588

C3 7.460352 0.144848 -5.002758

C4 4.164880 1.700345 -5.186791

C5 4.931521 -0.042256 -3.706340

H6 7.752209 0.206724 -3.951594

H7 7.125144 -0.868834 -5.233474

C8 8.657336 0.494788 -5.875048

C9 2.888437 1.585037 -4.666901

H10 4.385979 2.417950 -5.967156

H11 5.707103 -0.686655 -3.317249

C12 3.638544 -0.155571 -3.172697

O13 9.259828 1.668633 -5.367144

H14 8.322699 0.639993 -6.906866

H15 9.365815 -0.338555 -5.848993

C16 2.616620 0.656327 -3.651068

H17 2.083345 2.213426 -5.027117

H18 3.461224 -0.872354 -2.379491
C19 10.388979 2.090039 -6.112915
O20 1.330554 0.628257 -3.196450
H21 11.087798 1.259467 -6.251901
H22 10.079931 2.458161 -7.095810
C23 11.093254 3.205313 -5.351746
C24 1.071846 -0.028520 -1.960156
O25 11.723772 2.641195 -4.217552
H26 10.362616 3.963216 -5.051781
H27 11.833966 3.672365 -6.008726
C28 -0.293000 0.473854 -1.478621
H29 1.050043 -1.112637 -2.088224
H30 1.849616 0.234788 -1.242939
C31 12.429014 3.580025 -3.427504
O32 -0.641669 -0.143763 -0.257867
H33 -1.059553 0.197807 -2.201341
H34 -0.265087 1.560077 -1.375634
H35 13.217174 4.063832 -4.013560
H36 11.749396 4.349818 -3.049776
C37 13.062143 2.843524 -2.255142
C38 -0.002319 0.385722 0.890697
O39 12.028641 2.333121 -1.433104
H40 13.691164 3.542168 -1.694462
H41 13.688818 2.028469 -2.629821
C42 0.015251 -0.737599 1.918227
H43 1.023188 0.687629 0.673818
H44 -0.538646 1.259983 1.267722

C45 12.500469 1.656839 -0.284822
O46 0.815462 -0.326492 3.013035
H47 0.428486 -1.631093 1.443764
H48 -1.005639 -0.959550 2.246319
H49 13.179993 0.846213 -0.565620
H50 13.029365 2.344765 0.381677
C51 11.306233 1.056428 0.440628
C52 0.931725 -1.339261 3.994741
O53 10.544387 2.122992 0.987545
H54 11.653613 0.392327 1.235438
H55 10.701859 0.491779 -0.270730
C56 1.834566 -0.862753 5.125304
H57 -0.055518 -1.582558 4.404024
H58 1.363122 -2.243187 3.554238
C59 9.353544 1.827436 1.584506
O60 3.202192 -0.847252 4.746656
H61 1.745198 -1.564949 5.954182
H62 1.516572 0.126050 5.465896
C63 8.844739 0.544009 1.747595
C64 8.622502 2.926005 2.061057
C65 3.645038 0.362710 4.157670
H66 9.395376 -0.323453 1.409870
C67 7.592259 0.352493 2.351293
C68 7.390387 2.737190 2.658087
H69 9.039065 3.918339 1.943624
C70 5.068257 0.106740 3.667271
H71 3.001472 0.649478 3.325798

H72 3.659819 1.165015 4.901527
H73 7.209226 -0.653835 2.450990
C74 6.855915 1.445927 2.785897
H75 6.812696 3.578615 3.021051
O76 5.594746 1.377084 3.309392
H77 5.047258 -0.561860 2.806081
H78 5.665668 -0.333743 4.468893
N79 2.880585 -4.216284 0.093896
C80 2.079874 -4.302000 1.224101
C81 2.247196 -3.947530 -1.113624
C82 4.299658 -3.911980 0.206476
H83 2.602957 -4.555342 2.137948
C84 0.745918 -4.122084 1.194682
C85 0.922391 -3.755068 -1.219087
H86 2.900268 -3.930537 -1.977539
C87 4.569687 -2.406627 0.139975
H88 4.660996 -4.324228 1.148927
H89 4.834725 -4.410404 -0.603795
H90 0.204695 -4.265364 2.119332
C91 0.034559 -3.746247 -0.042788
H92 0.520507 -3.608702 -2.211537
C93 5.775838 -1.920229 -0.375379
C94 3.607826 -1.493251 0.570895
C95 -1.281913 -3.400755 -0.095708
C96 6.007089 -0.549454 -0.466287
H97 6.530846 -2.618262 -0.721690
H98 2.661768 -1.843312 0.969508

C99 3.842944 -0.121505 0.476387
C100 -2.168502 -3.354486 1.078428
C101 -1.977161 -3.013486 -1.334355
C102 5.035222 0.365991 -0.054155
H103 6.944829 -0.185481 -0.874366
H104 3.080935 0.570298 0.813937
H105 -1.794551 -3.609144 2.060127
C106 -3.457044 -2.977153 0.988922
C107 -3.274639 -2.660799 -1.347425
H108 -1.452083 -2.995879 -2.278230
C109 5.283433 1.866145 -0.206864
N110 -4.067856 -2.650991 -0.210202
H111 -4.096796 -2.918965 1.860584
H112 -3.777092 -2.361175 -2.258594
N113 4.062923 2.654955 -0.150412
H114 5.755161 2.047120 -1.172239
H115 5.963655 2.209186 0.573977
C116 -5.292747 -1.866121 -0.206333
C117 3.293253 2.789106 -1.293551
C118 3.442286 2.889534 1.065049
H119 -5.834197 -2.063174 -1.133413
H120 -5.916784 -2.205230 0.621805
C121 -5.023697 -0.364087 -0.077869
C122 2.005822 3.179110 -1.274796
H123 3.807818 2.565740 -2.219133
H124 4.069479 2.731562 1.934794
C125 2.152141 3.262633 1.167687

C126 -6.090546 0.543541 -0.050850
C127 -3.722852 0.123873 -0.005293
C128 1.290766 3.449492 -0.014502
H129 1.503332 3.260555 -2.227603
H130 1.762529 3.426781 2.162256
H131 -7.111002 0.178205 -0.110086
C132 -5.853780 1.911397 0.044337
C133 -3.488342 1.497972 0.085813
H134 -2.866028 -0.540784 -0.032976
C135 -0.024242 3.804051 0.048927
H136 -6.690878 2.602401 0.059876
C137 -4.544062 2.403808 0.113019
H138 -2.464632 1.848599 0.125077
C139 -0.872766 4.017628 -1.138855
C140 -0.773097 3.984154 1.306958
C141 -4.290344 3.911955 0.206723
C142 -2.202750 4.189478 -1.045389
H143 -0.436712 4.046076 -2.127542
H144 -0.263313 3.974542 2.259131
C145 -2.108685 4.150143 1.321749
N146 -2.874283 4.241835 0.167611
H147 -4.708570 4.302279 1.136010
H148 -4.788436 4.418814 -0.622024
H149 -2.827459 4.318471 -1.920850
H150 -2.663216 4.243071 2.247617

5. References

- S1.** (a) Odell, B.; Reddington, M. V.; Slawin, A. M. Z.; Spencer, N.; Stoddart, J. F.; Williams, D. *J. Angew. Chem. Int. Ed. Engl.* **1988**, 27, 1547–1550. (b) Sue, C.-H.; Basu, S.; Fahrenbach, A.; Shveyd, A. K.; Dey, S. K.; Botros, Y. Y.; Stoddart, J. F. *Chem. Sci.* **2010**, 1, 119–125. (c) Barnes, J. C.; Juriček, M.; Vermeulen, N. A.; Dale, E. J.; Stoddart, J. F.; *J. Org. Chem.* **2013**, 78, 11962–11969.
- S2.** (a) Helgeson, R. C.; Tarnowski, T. L.; Timko, J. M.; Cram, D. J.; *J. Am. Chem. Soc.* **1977**, 99, 6411–6418. (b) Anelli, P.-L.; Ashton, P. R.; Ballardini, R.; Balzani, V.; Delgado, M.; Gandolfi, M. T.; Goodnow, T. T.; Kaifer, A. E.; Philp, D.; Pietraszkiewicz, M.; Prodi, L.; Reddington, M. V.; Slawin, A. M. Z.; Spencer, N.; Stoddart, J. F.; Vicent, C.; Williams D. J. *J. Am. Chem. Soc.* **1992**, 114, 193–218.
- S3.** Hamilton, D. G.; Davies, J. E.; Prodi, L.; Sanders, J. K. M. *Chem. Eur. J.* **1998**, 4, 608–620.
- S4.** (a) Ashton, P. R.; Brown, C. L.; Chrystal, E. J. T.; Goodnow, T.; Kaifer, A. E.; Parry, K. P.; Philp, D.; Slawin, A. M. Z.; Spencer, N.; Stoddart, J. F.; Williams, D. J. *J. Chem. Soc., Chem. Commun.* **1991**, 9, 634–639. (b) Miljanić, O. Š.; Stoddart, J. F. *Proc. Natl. Acad. Sci. USA* **2007**, 104, 12966–12970.
- S5.** Ashton, P. R.; Goodnow, T. T.; Kaifer, A. E.; Reddington, M. V.; Slawin, A. M. Z.; Spencer, N.; Stoddart, J. F.; Vicent, C.; Williams, D. J. *Angew. Chem. Int. Ed. Engl.* **1989**, 28, 1396–1399.
- S6.** D. Jacquemin, V. Wathelet, E. A. Perpète, C. Adamo, *J. Chem. Theory Comput.* **2009**, 5, 2420 – 2435.
- S7.** Hartlieb, K. J.; Liu, W.-G.; Fahrenbach, A. C.; Blackburn, A. K.; Frasconi, M.; Hafezi, N.; Dey, S. K.; Sarjeant, A. A.; Stern, C. L.; Goddard, W. A.; Stoddart, J. F., *Chem. Eur. J.* **2016**, 22 (8), 2736-2745.

S6. Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kuš, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyayev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt, A.; Stein, T.; Stück, D.; Su, Y.-C.; Thom, A. J. W.; Tsuchimochi, T.; Vanovschi, V.; Vogt, L.; Vydrov, O.; Wang, T.; Watson, M. A.; Wenzel, J.; White, A.; Williams, C. F.; Yang, J.; Yeganeh, S.; Yost, S. R.; You, Z.-Q.; Zhang, I. Y.; Zhang, X.; Zhao, Y.; Brooks, B. R.; Chan, G. K. L.; Chipman, D. M.; Cramer, C. J.; Goddard, W. A.; Gordon, M. S.; Hehre, W. J.; Klamt, A.; Schaefer, H. F.; Schmidt, M. W.; Sherrill, C. D.; Truhlar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J.-D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C.-P.; Jung, Y.; Kong, J.; Lambrecht, D. S.; Liang, W.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Van Voorhis, T.; Herbert, J. M.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M., *Mol. Phys.* **2015**, *113*, 184-215.